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Pollutants from Synthetic Fuels Production Coal Gasification Screening Test Results

Research Triangle Inst.
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Prepared for

Industrial Environmental Research Lab.
Research Triangle Park, NC

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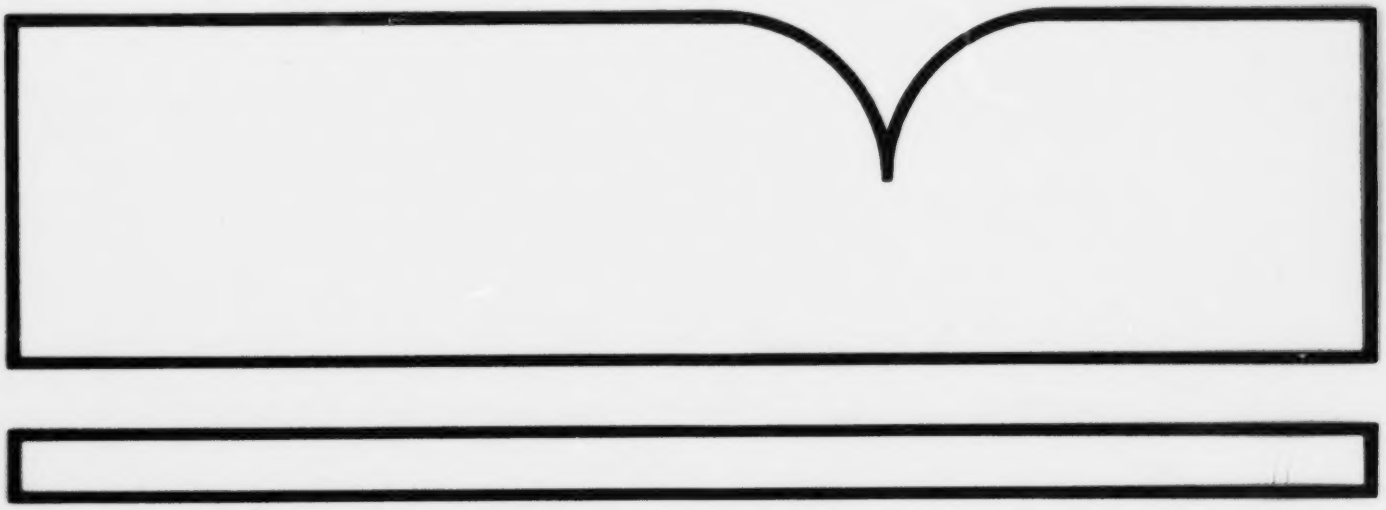

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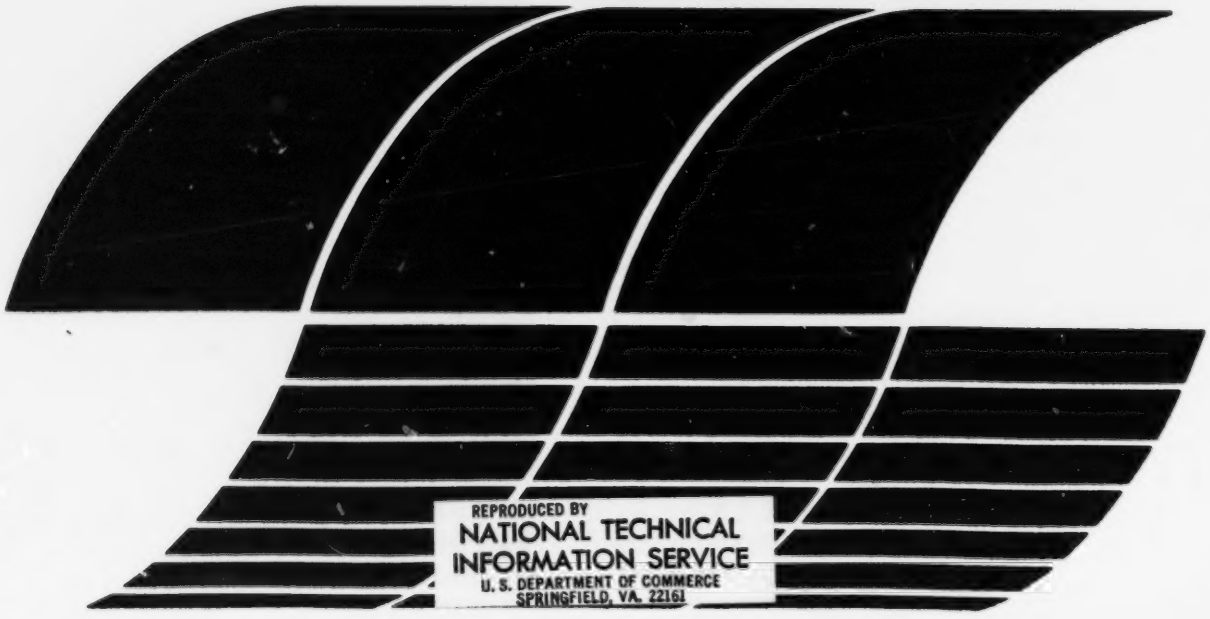
Interagency Energy/Environment R&D Program Report



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Pollutants from Synthetic Fuels Production: Coal Gasification Screening Test Results

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POLLUTANTS FROM SYNTHETIC FUELS PRODUCTION:
COAL GASIFICATION SCREENING TEST RESULTS

ABSTRACT

Coal gasification test runs have been conducted in a semibatch, fixed-bed laboratory gasifier in order to evaluate various coals and operating conditions for pollutant generation. Thirty-eight tests have been completed using char, coal, lignite, and peat. Reactor temperatures ranged from 790°C to 1035°C with high carbon and sulfur conversions in the bed.

Extensive analyses were performed for organic and inorganic compounds and trace elements in the tars and hydrocarbon oils, aqueous condensates, and reactor residues resulting from the gasification tests. Over 300 compounds were identified from the various gasifier streams, and more than 100 of these compounds were quantified for several of the test runs.

Statistical analyses have been performed on the data. The quantity and composition of the various effluents have been examined in relation to coal type and operating variables. Results are reported for sulfur species in the product gas stream, for consent decree pollutants contained as volatile organic compounds in the product gas, for phenol and related compounds in the aqueous condensate and tar/oil sample, and for polynuclear aromatic hydrocarbons (PNA) species in the tar/oil.

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Mr. Fred Schwarz of the Process Engineering Department manufactured and fabricated essentially the complete gasification facility in the RTI machine shop. His insights and handiwork gave rise to functional and productive hardware.

1.0 INTRODUCTION

This project is being conducted by the Research Triangle Institute in order to develop an understanding of the nature and extent of the production of environmental pollutants in synthetic fuels processes. Screening test runs have been conducted in a laboratory scale nonisothermal reactor. Eight distinct coals or related materials have been gasified under various operating conditions so as to screen the pollutants produced by a variety of feed materials considered to be candidates for coal gasification within the United States.

A report on the facility construction and preliminary tests was previously prepared.[1] That report described the design and construction of the gasification facility including the reactor and associated feed devices, the sampling and analysis system development, and the on- and off-line data collection and evaluation capability. (See Figure 1).

Some 38 gasification tests were conducted in order to (1) establish the range of operating conditions over which the laboratory reactor can be successfully operated, (2) establish the operating characteristics of the gasifier and ascertain the extent to which its results match those of large scale units, (3) conduct extensive chemical analysis work aimed at the identification of the chemical species in the various effluents from the gasifier, (4) complete approximate quantitative analyses on the gasifier effluents which are present in sufficient quantities to be environmentally significant, and (5) establish operating conditions for parametric studies. The fossil fuel sources which have been gasified include FMC char, Illinois No.6 coal, Western Kentucky No.9 coal, Pittsburgh No.8 coal, Montana Rosebud coal, Wyoming subbituminous (Smith-Roland) coal, North Dakota Zap lignite, and North Carolina humus peat. These tests have been conducted both with externally supplied heat as well as with heat derived from partial combustion taking place as a part of the overall gasification process.

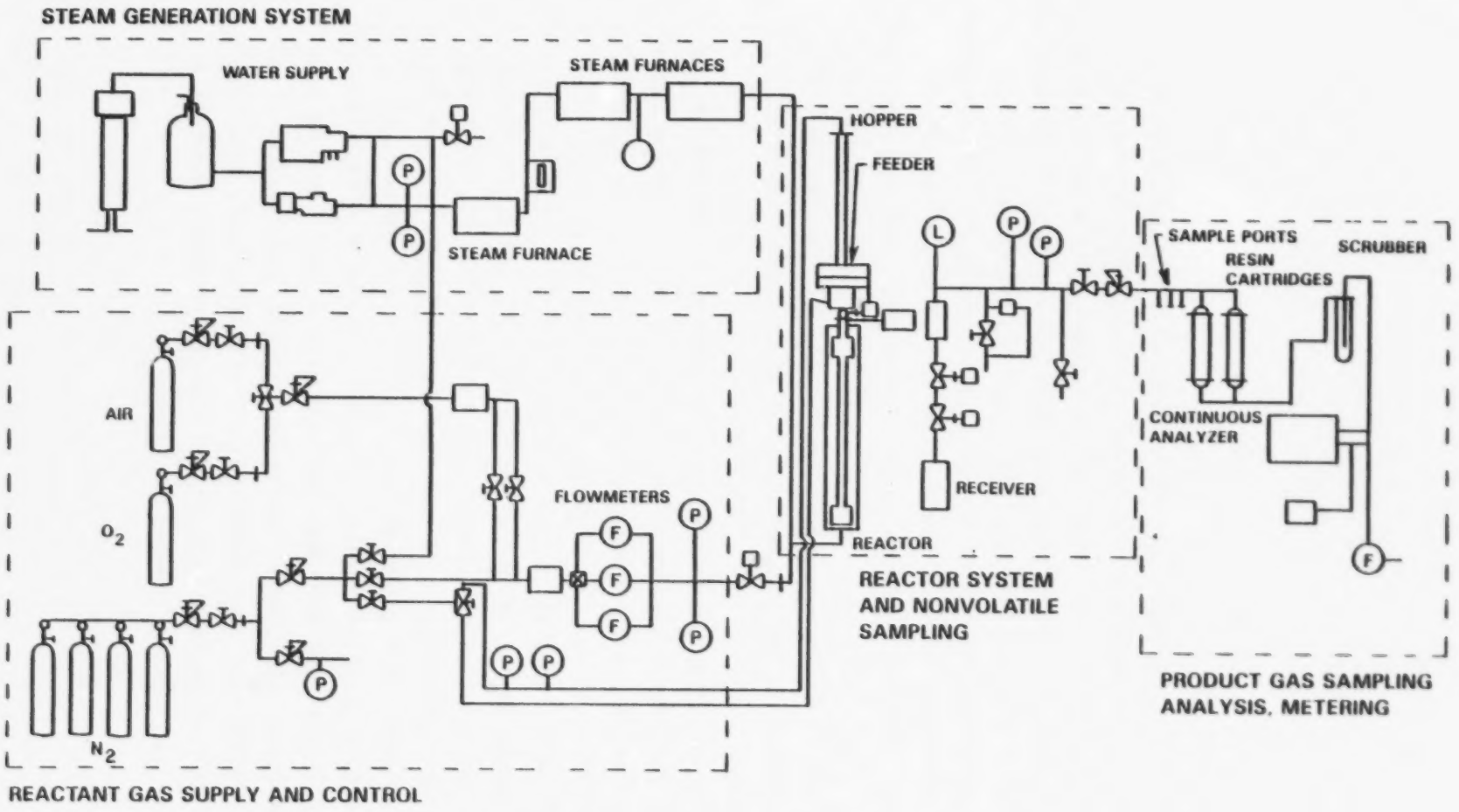

Figure 1. Gasifier and sampling train.

Operating conditions have been chosen in many cases to approximate those of large scale gasifier operations producing low heating value fuel gas or synthesis gas. However, coal addition has been by way of batch addition to the reactor from a pressurized lockhopper. Thus, the coal feed has been a batch process while the addition of air and/or steam to the reactor has involved continuous flow throughout a gasification test run. Hence, operation of the reactor during the screening tests is referred to as being in the semibatch fixed-bed mode.

If the effluent concentrations for a semibatch run are averaged by integration over the time of the run to simulate the steady-state concentrations of a continuous process, then the semibatch reactor produces effluent concentrations which appear to provide a reasonably good simulation of gas product compositions from full scale process gasifiers. Where comparative results are available, the results obtained in this study have shown good agreement for such major pollutants as sulfur compounds, phenols, total organics, benzene derivatives, and total tar.

Companion reports are simultaneously being prepared and issued on (1) the sampling and analysis methodology which has been developed for use in this project and (2) the health and environmental significance of the results which have been obtained from the screening tests.[2,3] Separate reports are also planned on related topics. One is intended on the transient behavior of the gasification test runs relative to both reactor operation and the concentration of effluents. Another is to be a comparison of the results of this study with the available comparative data on pilot plant and commercial gasification operations.

Future reports will also present information relative to parametric studies, which examine the generation and control of potential pollutants in coal gasification under various operating conditions. The parameters under consideration are coal type, coal particle size, reactant flow rates, chemical additives, and other factors. Information being generated in this project is intended to provide a basis for the assessment of the potential health and environmental significance of the effluents from coal gasification processes. The project results should also lead to process modifications and/or control technology developments which permit substantial reductions in potential emissions.

2.0 SCREENING TEST CONDITIONS

Screening tests have been completed using selected coals, lignite, peat, and a coal-derived char. Semibatch fixed-bed gasification was conducted to generate, collect, process, analyze, characterize, and evaluate the pollutants from the gasification of each feed material. Flow rates of steam and/or air were predetermined for each run so as to achieve desired reaction temperatures. Additionally, external furnaces were utilized to control the temperatures and heating rates involved. An on-line signal processing system was utilized to collect process data, to collect and analyze gas chromatograph output signals, and to perform overall data processing functions. This PDP 11/34 system and associated equipment and software are described in an appendix.

2.1 FOSSIL FUELS GASIFIED

The eight distinct fossil fuel sources which have been studied during the screening tests are presented in Table 1. These coals and related materials have been subjected to determinations of free swelling index, heating value, ultimate analysis, proximate analysis, sulfur species, and ash fusion temperature. These values are typical or representative of the various coal seams from which the samples were obtained. (It is known that the moisture content as well as other possible parameters for a particular coal type can vary from one sample to another. Representative analyses, as shown in Table 1, were used for the screening test studies. However, individual analyses for the particular feed material utilized for each gasifier test run are being performed for the feed materials in the parametric test runs of this research program).

2.2 REACTOR OPERATING CONDITIONS

The air-to-coal ratio, steam-to-coal ratio, reactor pressure and temperature were selected for many of the screening tests in order to obtain conditions comparable to those used in pilot plant or commercial coal gasification

TABLE 1. ANALYSIS OF FUELS GASIFIED

Fuel	Btu/lb (inc. moisture & ash)	Moisture %	Ash %	Volatile Matter %	Fixed Carbon %	Sulfur: Sulfate / Organic / Pyritic / Total	Carbon %	Hydrogen %	Oxygen %	Nitrogen %	FSI %	Ash Fusion Temp. °F
W. Kentucky FMC Char	11,090	1.90	19.70	7.80	71.50	1.80	74.02	1.48	1.70	1.3	<1.0	2600*
Illinois No. 6 Bituminous	11,331	6.85	13.52	32.58	47.05	0.15 / 1.16 / 1.71 / 3.02	63.26	5.37	13.46	1.35	3.5	2350°F** (2030-2730°F) 2280*
Montana Rosebud Subbituminous	9,004	21.19	8.86	31.56	38.39	0.17 / 0.21 / 0.21 / 0.59	53.95	6.87	28.53	1.20	0.0	(2150-2240°F)
N.C. Humus Peat	4,975	45.98	3.67	31.81	18.54	0.05 / 0.06 / 0.01 / 0.12	30.22	5.34	59.84	0.81	0.0	
Pittsburgh No. 8	12,288	3.08	11.09	29.16	56.67	<0.01 / 1.28 / 1.24 / 2.53	72.29	3.45	8.62	1.95	7	2270°F** (2060-2780°F)
Wyoming Subbituminous	7,880	15.56	6.31	38.30	39.30	0.07 / 0.08 / 0.40 / 0.55	56.80	5.94	30.02	0.38	0	2280°F* (2110-2460°F)
N. Dakota Lignite	7,880	29.63	6.39	28.57	35.41	0.01 / 0.54 / <0.01 / 0.56	46.82	9.85	35.63	0.73		2340°F**
W. Kentucky No. 9 Bituminous	12,130	7.03	7.83	38.78	46.36	0.05 / 2.90 / 1.83 / 4.78	67.36	5.58	13.68	1.08	4	2090°F** (1970-2400°F)

*As received--%H and %O include that portion in moisture.
**Mean temperature

reactors. Table 2 presents various experimental test conditions for the RTI tests in relation to selected gasifier operating conditions. While the air-to-coal ratio is generally lower for the RTI tests, most of the conditions which have been examined have shown a quite close correspondence to those for pilot scale and commercial fixed-bed gasification processes.

Actual quantities of coal, steam, air, and tar involved in various screening tests are presented in Table 3. Steam-to-carbon ratios have been investigated over the range from 0.4 to 18 g/g and air-to-carbon ratios from 0 to about 4 g/g. Although the air-to-coal ratio has varied depending upon the intended method of supplying heat to the reactor, the steam-to-coal ratio has been predominantly in the range of 0.5 to 3.0 g/g. (Excessive steam simply passes through the reactor and results in additional aqueous condensate formation in the reactor condenser system). Maximum bed temperatures have been in the range of 900 to 1000°C. Carbon conversions have ranged from 52 to near 100 percent, oxygen-to-coal ratios from 0.0 to 0.9 g/g, and steam-to-oxygen ratios from 0.9 to infinite. Both internal and external heat has been supplied to the reactor system.

2.3 EFFLUENT SAMPLING AND CHEMICAL ANALYSIS

The effluent gas stream from the fixed-bed reactor passes through a particulate trap which is insulated to maintain hot gas conditions. This is immediately followed by a refrigerated condenser unit which removes aqueous condensate and low volatile organic material at the system pressure. The condenser unit is followed by a backpressure regulator.

A glass sampling system has been installed on the low pressure side of the backpressure regulator. This system includes ports for grab samples and a valving system for direct adsorbent cartridges. A port also exists for removal of a continuous gas stream for infra-red analysis. Further, the primary gas stream passes through a continuous dry gas meter to measure the total volumetric flow of the effluent stream.

Raw gas samples were collected periodically during the gasification test. These samples were contained in special glass sample bulbs and maintained under controlled conditions in a specially designed sample storage chest.

TABLE 2. EXPERIMENTAL TEST PARAMETERS AND COMMERCIAL GASIFIER OPERATING CONDITIONS

	RTI Tests						METC[4]	Lurgi[5,6]	Wellman Galusha[5]	Woodall Duckham[5]
	21	23	25	32	33	35				
Air/Coal g/g	1.1	2.2	1.7	1.5	1.5	1.7	2.3	3.0	3.5	2.3
Steam/Coal g/g	3.1	1.2	0.50	0.37	0.36	0.37	0.31	1.5	0.4	0.25
Carbon Conversion %	97	96	99.7	99.5	98.9	97	98.7	95	99+	99
Coal Residence Time (min.)	340	300	180	110	110	110	120-540	60	120-540	NA
Tar Produced g/g	0.035	0.033	0.018	0.011	0.012	0.029	0.022	NA	0.06	0.075
Gas Produced SCF/lb	48	56	41	32	35	40	47	52	NA	NA
HHV Btu/SCF	106	96	142	183	201	128	153	195	168	175
Throughput lb/hr ft^2	16	19	30	44	45	46	107	248	899	70
Coal Type	Illinois No.6	Illinois No.6	Montana Subbit.	Wyoming Subbit.	Wyoming Subbit.	Wyoming Subbit.	Illinois No.6	Subbituminous C New Mexico	Bituminous	HVCB
Pressure psia	200	200	200	200	200	200	315	300	ATM	ATM
Mesh Size	8 x 16	8 x 16	8 x 16	8 x 16	8 x 16	8 x 16	2" x 0	1.75" x 0.08"	2" x 1.25"	1.5" x 0.25"
Maximum Temperature °C	1015	1050	1060	1050	1040	910	--	--	1300	1200
Heatup Time to 800°C (min.)	20	11	3	5	8	23	--	--	--	--
Gas Composition										
CO	16	10	24	29	32	16	21.8	17.4	28.6	28.3
CO_2	18	18	9.1	9.1	4.9	12	6.9	14.8	3.4	4.5
CH_4	5.4	3.1	2.4	5.7	5.7	3.7	2.0	5.1	2.7	2.7
H_2	30	13	13	20	20	14	17.8	23.3	15.0	17.0
N_2	30	55	52	36	37	54	51.5	38.5	50.3	47.2
H_2S	0.4	0.8	0.06	0.07	0.07	0.08	0.2	NA	NA	0.3
HHV Btu/SCF	200	100	140	210	210	130	150	200	170	170

TABLE 3. OPERATING CONDITIONS--SCREENING TESTS

Test / Coal	RTI Test Number								
	16 Illinois No.6	21 Illinois No.6	23 Illinois No.6	41 Western Kentucky	25 Montana	33 Wyoming	35 Wyoming	36 North Dakota	43 North Dakota
Steam (g)	3704	4713	1952	1390	748	500	527	639	422
Air (g)	1350	1720	3288	3060	2482	2097	2461	1939	2022
Coal (g)	1569	1543	1594	1250	1491	1396	1420	1444	1458
Air/Coal	0.86	1.1	2.1	2.5	1.7	1.5	1.7	1.3	1.4
Steam/Coal	2.4	3.1	1.2	1.1	0.50	0.36	0.37	0.44	0.29
Air/Steam	0.35	0.35	1.8	2.2	3.4	4.2	4.6	3.1	4.8
T_{max}* °C	941	984	1020	1034	1006	1010	790	916	914
Carbon Conversion (%)	89	97	96	99.8	99.7	98.9	97	99.7	99.4
Sulfur Conversion (%)	93	98	95	98	85	91	85	91	80
Tar Yield (g/g Coal)	0.036	0.033	0.033	0.030	0.018	0.012	0.029	0.013	0.0072

*Time averaged maximum bed temperature.

These samples were systematically subjected to gas chromatographic analysis for a range of specific compounds including ethane, ethylene, and acetylene; benzene, toluenes, and xylenes; hydrogen sulfide, carbonyl sulfide, and other sulfur species. Moreover, a continuous gas monitor was utilized in all screening tests in order to obtain a continuous analysis for methane, carbon monoxide, carbon dioxide, and hydrogen.

The adsorbent cartridges have utilized XAD-2 resins for the volatile organic constituents. A single cartridge was used throughout the initial portion of the run, the so-called surge period. A valving arrangement permitted switching of the cartridge to a fresh resin for utilization during the so-called steady-state period, which presumably represents primarily the char gasification process. These XAD-2 resins were extracted with methylene chloride; the extracts were subjected to GC/mass spectrometer analysis.

The condensate collection container was drained periodically throughout a run with the content being accumulated for a complete gasification test. This mix of aqueous condensate and low volatile organic material was subjected to phase separation followed by a detailed chemical partitioning process. The aqueous phase was extracted with methylene chloride to remove residual organic constituents. The low volatile organic phase was extracted so as to obtain tar acids, tar bases, polar neutrals, nonpolar neutrals, PNA, and hexane insoluble chemical constituents.[2]

The effluents from screening test runs have been subjected to a wide variety of chemical and bioassay tests in order to characterize and evaluate these materials.[3] Individual reports have been prepared on the sampling and analysis scheme as well as the environmental/health aspects of the results which have been obtained.[2,3] Additional reports are under preparation to describe the results of parametric runs using the fixed-bed coal gasification unit.

3.0 EXPERIMENTAL RESULTS

Chemical analysis results have been obtained for the raw gas bulb samples, the XAD-2 adsorbent resin samples, the low volatile organic material (tar), the aqueous condensate, and bottom ash, which remained within the reactor. The results include continuous monitor values for four primary gases, GC analyses for a variety of hydrocarbon and sulfur species gases, GC/MS analyses for volatile and low volatile organic compounds, plus a variety of elemental determinations by atomic absorption and other techniques.

3.1 REACTOR SYSTEM BEHAVIOR

A detailed examination of the temperature profiles throughout various screening test runs was completed. These results indicate that (1) the initial temperature distribution undergoes considerable modification early in a run (surge period) but maintains a common character throughout the steady-state period in most cases, and (2) severe temperature gradients occur at or near the top of the fixed-bed of solids throughout a run. The surge period is generally of relatively short duration, e.g., 20 minutes, and is indicated by that period over which the methane concentration in the raw effluent gas is 2 percent, by volume, or greater. Thus, reasonably uniform temperature control was obtained over the duration of the char gasification process (steady-state period).

Results that have been obtained with various coals in the RTI gasification tests indicate that the degree of desulfurization during partial gasification is always higher than the carbon conversion. Sulfur in the resulting gas is present mainly in the form of hydrogen sulfide. Recent research[7] conducted in Germany has also indicated that during the gasification of coal at temperatures about 950°C, rapid degassing takes place which involves desulfurization of the coal, with up to 55 percent of the sulfur being removed in the first four seconds. The resulting material is a coke or char which reacts with oxygen and/or steam to produce carbon monoxide, carbon dioxide, and hydrogen.

Raw gas analyses indicate a decrease in hydrogen sulfide concentration with time followed typically by a period of level (constant) concentration, or in some cases, an increase. Carbonyl sulfide concentrations were found

generally to initially decrease and then level off or follow the H_2S pattern. These concentrations of carbonyl sulfide generally were found to be between one to two orders of magnitude lower than those for the hydrogen sulfide. Methanethiol and thiophene concentrations for all tests were found to undergo an early decrease from an initial maximum value to levels below the detection limits of the gas chromatograph being utilized, i.e., below 1 ppm by volume.

Additional work is, of course, needed in elucidating the mechanisms for the formation of sulfur species. It is generally believed that pyritic compounds give rise to hydrogen sulfide under the reducing conditions typical in coal gasification processes. Other sulfur compounds such as methanethiol, ethanethiol, thiophene, etc., may well result from the decomposition of organically bound sulfur in the coal material. An additional consideration is that elemental sulfur may well exist in the gas phase.

Considering the behavior of the lower sulfur coals tested, the surge phase levels of volatile organic sulfur compounds, e.g., methanethiol and thiophene, are found to be much lower than those for the high sulfur Illinois No.6 coal. For reactive coals, e.g., Wyoming subbituminous and Montana Rosebud, the levels of devolatilized organic sulfur compounds were reduced to lower than minimum detectable levels as measured with an FPD detector on the GC within less than 15 minutes from the introduction of the coal into the reactor. Ninety percent or more of the C_6-C_8 aromatics also evolved during the first 15 minutes of these tests.

Concentration of the inorganic sulfur compounds H_2S and COS were generally found to follow the CO_2 concentration. These concentrations reached a minimum about midway during the tests carried out over 1000°C, but decreased monotonically for tests carried out at lower temperatures (900°C). In some cases the concentrations of H_2S and COS were found to increase near the end of a run, indicating that relatively inactive sulfur-containing compounds in the reactor were being converted after almost all of the carbon content had been converted.

The residue (bottom ash) analyses for various screening test runs are presented in Table 4. These values indicate that substantial carbon conversions were obtained in almost all of the screening test runs. Sulfur conversions generally were not as high, indicating that while there may be char species

TABLE 4. RESIDUE (BOTTOM ASH) ANALYSES

	RTI Test Number								
	16	21	23	25	33	35	36	41	43
Volatile Matter %	2.04	4.80	6.58	5.88	9.94	2.00	1.59	2.76	14.38
Fixed Carbon %	34.46	11.14	10.37	-	9.76	26.76	2.66	0.10	-
Moisture %	0.15	0.46	0.68	0.66	2.58	2.53	3.76	0.11	4.69
Ash %	63.35	83.60	82.37	96.50	77.72	68.71	91.99	97.03	88.51
C %	35.90	14.51	15.57	1.77	15.28	24.81	2.52	1.64	5.24
H %	0.29	0.43	0.52	0.20	1.19	0.71	0.15	0.02	1.63
N %	0.32	0.53	0.57	0.06	0.14	0.31	0.06	0.08	0.00
S %	1.06	0.43	0.92	1.16	1.20	1.28	1.03	0.88	2.21
Cl %	NA	< 0.01	NA	NA	0.05	0.03	0.08	0.04	0.09
O (difference) %	-	0.04	-	-	1.84	1.62	0.41	0.20	-
Organic Sulfur %	NA	0.24	0.40	0.07	1.04	0.86	0.15	0.83	0.44
Pyritic Sulfur %	NA	0.09	0.25	0.04	0.15	<.01	0.80	0.03	0.06
Sulfate Sulfur %	NA	0.10	0.27	1.05	0.01	0.42	0.08	0.02	1.71
Heating Value (Btu/lb.)	3890	1990	2263	≤ 50	2700	3933	309	340	544
F.S.I..	0	0	0	0	1/2	NA	1/2	1/2	NA

NOTE: NA = Not Analyzed.
C and H are exclusive of moisture.

possessing relatively low reactivity carbon, the residual sulfur compounds are quite resistant to gasification. This is particularly true for sulfur which has been oxidized to, or originally was, sulfate sulfur. It is of interest to note, that in almost every case the organic sulfur content also exceeded the sulfate sulfur level within the reactor residue. The two exceptions are for runs 25 and 43 which involved Montana Rosebud and North Dakota lignite feed materials, respectively. (The individual carbon conversion and sulfur conversion values for each of the runs shown in Table 4 can be found in Table 3).

3.2 CHEMICAL ANALYSIS RESULTS

The gas chromatograph/mass spectrometer analysis of the various samples and extracts (partitions) obtained from the sampling and analysis programs associated with the gasification tests have resulted in the identification of more than 300 organic species. Additional compounds have been quantitated by direct gas chromatographic analysis. Atomic absorption measurements have been performed on the various effluents to determine trace element compositions.

Special attention has been given to compounds which were judged to have environmental significance with less attention being paid to organic species which currently available information indicates as being harmless. Criteria utilized for the analysis of screening test samples for this selectivity were twofold: first, compounds were specifically selected for study if they possessed moderately toxic to severe health hazard potentials as evidenced by a toxic threshold value less than 17 mg/m^3 and were suspected to occur in the gasifier effluents; and secondly, <u>any</u> compound present in the effluents at concentrations of 5 mg/m^3 or greater was given consideration. The list of compounds which have been detected throughout the screening test sequence is provided in Table 5. (It should be noted that some of the compounds listed were detected only in the aqueous condensate which was collected from the condenser unit on the effluent stream. The compounds thus identified may have been formed as a result of reaction of precursors in the condenser system.)

The quantity of selected compounds produced in various of the screening test runs per unit mass of carbon converted in the gasifier is presented in Table 6. It may be noted that the sulfur species and phenolic type compounds

TABLE 5. COMPOUNDS IDENTIFIED IN GASIFIER EFFLUENTS (Arranged by MEG Category)

MEG Category	Name
1.	Aliphatic Hydrocarbons
	methane
	ethane
	propane
	n-butane
	isobutane
	n-pentane
	isopentane
	n-hexane
	2-methylpentane
	3-methylpentane
	n-heptane
	n-octane
	n-nonane
	n-decane
	n-undecane
	n-dodecane
	n-tridecane
	n-tetradecane
	n-pentadecane
	n-hexadecane
	methylcyclobutane
	cyclopentane
	cyclohexane
	dimethylcyclohexane
	trimethylcyclohexane
	cyclooctane
	dimethyldecahydronaphthalene
	ethene
	propene
	butene
	isobutene
	hexene
	1-pentene
	2-methyl-1-butene
	1,3-butadiene
	pentadiene
	cyclopentene
	cyclohexene
	cyclopentadiene
	ethyne
	propyne
2.	Alkyl Halides
	dichloromethane(artifact)
	trichloromethane(artifact)
	carbon tetrachloride (artifact)
3.	Ethers
	diethylether
	phenyl-2-propynylether
	1-methoxynaphthalene
	2-methoxynaphthalene
	3,6-dimethoxyphenanthrene
	2-methoxyfluorene
5.	Alcohols
	3,5,5-trimethyl-1-hexanol
7.	Aldehydes, Ketones
	acetaldehyde.
	butanal
	pentanal
	p-hexanal
	n-heptanal
	n-octanal
	n-nonanal
	undecanal
	dodecanal
7.	(Continued)
	benzaldehyde
	dimethylbenzaldehyde
	acetone
	methylisopropyl ketone
	butanone
	1-phenyl-1-propanone
	2-pentanone
	acetophenone
	o-hydroxyacetophenone
	m-hydroxyacetophenone
	benzophenone
	9-fluorenone
	benzofluorenone
	dihydroxyanthraquinone
	tetrahydroanthraquinone
	phenanthridone
8.	Carboxylic Acids and Derivatives
	acetic acid
	benzoic acid
	benzamide
	ethyl acetate
	ethylbenzyl acetate
	methyl benzoate
	isobutyl cinnamate
	dibutyl phthalate(artifact)
	diisobutyl phthalate (artifact)
	dicyclohexyl phthalate (artifact)
9.	Nitriles
	acetonitrile
	cyanobutadiene
	benzonitrile
	2,2'-dicyanobiphenyl
10.	Amines
	aniline
	diphenylamine
	benzidine
	1-aminonaphthalene
	N-methyl-o-toluidine
13.	Thiols, Sulfides, and Disulfides
	methanethiol
	ethanethiol
	2,3,4-trithiapentane
	dimethyl sulfide
	dimethyl disulfide
	trithiahexane
	diphenyl disulfide
15.	Benzene, Substituted Benzene Hydrocarbons
	benzene
	toluene
	o-xylene
	m-xylene
	p-xylene
	ethylbenzene
	styrene
	methylstyrene
	ethylstyrene
	n-propylbenzene
	isopropylbenzene
	1,2-dimethylbenzene
	t-butylbenzene
	n-pentylbenzene
15.	(Continued)
	3,5-dimethyl-1-isopropyl-benzene
	triethylbenzene
	o-ethyltoluene
	m-ethyltoluene
	trimethylbenzene
	1,2,4-trimethyl-benzene
	1,3,5-trimethylbenzene
	o-diethylbenzene
	m-diethylbenzene
	p-diethylbenzene
	methyltetrahydro-napnthalene
	dimethyltetra-hydronaphthalene
	trimethyltetra-hydronaphthalene
	1,2,3,4-tetrahydro-napnthalene
	5,8-dimethyl-1-n-octyl-1,2,3,4-tetrahydronapn-thalene
	1-methyl-4-n-heptyl-1,2,3,4-tetra-hydronaphthalene
	biphenyl
	methylbiphenyl
	3-methylbiphenyl
	diphenylmethane
	diphenylethane
	di(ethylphenyl) ethane
	stilbene(1,2 diphenylethene)
	methylphenylethyne
	diphenylethyne
	1,2-diphenylpropane
	dixylylethane
	o-terphenyl
	m-terphenyl
	p-terphenyl
	indan
	methylindan
	dimethylindan
	pentamethylindan
	indene
	methylindene
	methy-1-2,3-dihydro-indene
	dimethylindene
	trimethylindene
18.	Phenols
	phenol
	o-cresol
	m-cresol
	p-cresol
	o-ethylphenol
	m-ethylphenol
	p-ethylphenol
	isopropylphenol
	o-allylphenol
	m-phenylphenol
	2,3-xylenol
	2,4-xylenol
	2,5-xylenol
	2,6-xylenol

TABLE 5 (continued).

MEG Category	Name
18.	(Continued)
	3,4-xylenol
	3,5-xylenol
	3-methyl-6-ethylphenol
	2-methyl-4-ethylphenol
	4-tert-butyl-o-cresol
	di-t-butyl-4-ethylphenol
	trimethylphenol
	2-hydroxynaphthalene
	methylhydroxynaphthalene
	hydroxyfluorene
21.	Fused Polycyclic Hydrocarbons
	naphthalene
	cyclobutadibenzene
	1-methylnaphthalene
	methyldihydronaphthalene
	2-methylnaphthalene
	ethylnaphthalene
	isopropylnaphthalene
	1-methyl-7-isopropyl-naphthalene
	1,2-dihydro-3,5,8-trimethylnaphthalene
	2-benzylnaphthalene
	dimethylnaphthalene
	1,4-dimethylnaphthalene
	2,3-dimethylnaphthalene
	2,6-dimethylnaphthalene
	trimethylnaphthalene
	acenaphthene
	acenaphthylene
	methylacenaphthylene
	3-methylacenaphthylene
	anthracene
	9-methylanthracene
	ethylanthracene
	phenanthrene
	methylphenanthrene
	1-methylphenanthrene
	3-methylphenanthrene
	4,5-methylenephenanthrene
	propenylphenanthrene
	trans-9-propenylphenanthrene
	8-n-butylphenanthrene
	2,7-dimethylphenanthrene
	pyrene
	methylpyrene
	1,2-benzanthracene
	hexahydro-1,2-benzanthracene
	methyl-1,2-benzanthracene
	2,3-benzanthracene (naphthacene)
	3,4-benzophenanthrene
	methylbenzophenanthrene
	5,8-dimethyl-3,4-benzophenanthrene
	9,10-benzophenanthrene (triphenylene)
	1,2,3,4-tetrahydro-9,10-benzophenanthrene
	2-methyl-9,10-benzophenanthrene
	chrysene
	methylchrysene
	benzo(a)pyrene
	benzo(e)pyrene
	perylene
21.	(Continued)
	2-n-hexylperylene
	benzo(g,h,i)perylene
	dibenzo(a,h)anthracene
22.	Fused Non-Alternant Polycyclic Hydrocarbons
	fluorene
	methylfluorene
	1-methylfluorene
	dimethylfluorene
	fluoranthene
	1,2,3,4-tetrahydrofluoranthene
	benzo(a)fluorene
	benzo(b)fluorene
	benzo(b)fluoranthene
	benzo(k)fluoranthene
	indeno(1,2,3 cd) pyrene
23.	Heterocyclic Nitrogen Compounds
	pyrrole
	methylpyrrole
	pyridine
	methyl pyridine
	4-acetylpyridine
	dimethylpyridine
	trimethylpyridine
	2,4-dimethyl-6-ethylpyridine
	2-hydroxy-4-phenylpyridine
	2-hydroxy-6-phenylpyridine
	3,4-diphenylpyridine
	benzopyridine
	2,2'-dimethyl-4,4'-dipyridyl
	indole
	methylindole
	methyl-3-allylhydroindole
	3-methyl-3-allydihydroindole
	phenylindole
	3-methyl-2-phenylindole
	3,3'-biindolyl
	quinoline
	isoquinoline
	methylquinoline
	3-methylquinoline
	6-methylquinoline
	ethylquinoline
	3-n-propylquinoline
	4-n-propylquinoline
	8-n-propylquinoline
	dimethylquinoline
	2,6-dimethylquinoline
	methylphenylquinoxaline
	4-styrylquinoline
	7,8-benzoquinoline
	3-methylbenzoquinoline
	benzimidazole
	methylbenzimidazole
	2-ethylbenzimidazole
	benzylbenzimidazole
	benzothiazole
	2-methyl-5-phenyltetrazole
	diphenyloxazole
	acridine
	dimethylacridine
	acridone
	carbazole
	9-methylcarbazole
23.	(Continued)
	1,2,3,4-tetrahydrocarbazole
	3-amino-9-ethylcarbazole
	vinylphenylcarbazole
	1,4-dihydro-2,3-benzo(b)carbazole
	2-amino-4-phenyl-6-methylpyrimidine*
	2-amino-5-chloro-4,6-dimethylpyrimidine*
	4-(1,2,3,4-tetrahydro-2-naphthyl)-morpholine
	3-benzylindene phthalimide*
24.	Heterocyclic Oxygen Compounds
	furan
	benzofuran
	2-methylbenzofuran
	3-methylbenzofuran
	5-methylbenzofuran
	7-methylbenzofuran
	3,3-dihydro-2-methylbenzofuran
	dimethylbenzofuran
	3,6-dimethylbenzofuran
	dihydromethylphenylbenzofuran
	dibenzofuran
	xanthene
25.	Heterocyclic Sulfur Compounds
	thiophene
	2-methylthiophene
	3-methylthiophene
	2,3-dimethylthiophene
	2,4-dimethylthiophene
	2,5-dimethylthiophene
	3,4-dimethylthiophene
	trimethylthiophene
	isopropylthiophene
	ethylthiophene
	2-n-propyl-5-isobutylthiophene
	benzothiophene
	methylbenzothiophene
	dimethylbenzothiophene
	trimethylbenzothiophene
	benzodithiophene
	methylbenzodithiophene
	dibenzothiophene
	methyldibenzothiophene
	dihydrodimethylthienothiophene
	dimethylthiaindene
	thiaxanthene
42.	Carbon Compounds
	carbon monoxide
	carbon dioxide
47.	Nitrogen Compounds
	ammonia
	hydrogen cyanide
52.	Sulfur Compounds
	sulfur
	sulfur dioxide
	hydrogen sulfide
	carbonyl sulfide
	carbon disulfide
99.	Hydrogen
	hydrogen

TABLE 6. POLLUTANT PRODUCTION

$$\frac{(\mu g \text{ produced in all streams})}{g \text{ carbon converted}}$$

Compound	RTI Test Number								
	16	21	23	25	33	35	36	41	43
hydrogen sulfide	3.8E3	3.8E3	9.8E4	4.6E3	3.4E3	5.9E2	4.9E2	4.0E4	3.1E3
carbonyl sulfide	4.0E2	2.0E2	5.6E2	1.5E2	2.0E2	3.1E2	3.7E2	8.5E2	5.8E2
methanethiol	3.9E1	8.3E1	5.2E1	4.1E0	2.5E1	4.6E1	1.7E2	5.8E1	2.4E1
ethanethiol	-	-	2.1E0	-	-	-	1.4E2	-	-
carbon disulfide	7.8E1	4.9E1	2.5E2	-	-	-	-	1.1E0	1.4E1
thiophene	1.8E3	5.9E2	3.8E3	5.2E1	1.6E1	5.5E1	1.1E3	4.0E2	1.9E1
methylthiophene	3.2E2	1.0E3	1.1E3	1.1E1	1.8E2	5.5E1	2.9E1	4.9E2	7.6E1
hydrogen cyanide	-	1.3E2	-	1.2E2	-	-	1.4E2	-	-
ammonia	-	1.5E4	-	8.7E3	-	-	6.0E3	-	-
aniline	-	1.5E1	1.0E1	1.3E0	1.6E0	2.5E0	-	-	-
quinoline	-	1.7E2	1.3E2	9.5E1	1.8E1	6.3E0	2.5E1	4.9E1	3.9E0
acridine	-	9.1E1	8.1E1	2.5E0	4.3E0	1.8E0	1.8E1	2.1E1	-
indole	-	3.1E0	-	1.3E0	-	1.3E0	-	-	-
phenol	4.3E2	4.7E2	7.8E2	8.3E2	2.7E3	2.9E3	1.4E3	1.2E3	2.7E3
cresols	7.2E2	1.3E3	1.7E3	1.0E3	8.9E2	2.6E3	1.0E3	1.3E3	2.0E3
xylenols	-	7.4E2	7.6E2	1.9E2	3.1E3	2.3E3	1.1E3	2.9E2	4.1E3
trimethyl phenol	-	6.5E1	1.3E2	2.3E1	5.8E1	7.4E1	3.0E1	7.6E1	3.8E2
o-isopropyl phenol	-	-	1.3E2	-	2.0E1	3.3E1	8.9E0	3.2E1	4.5E1

Note: Ammonia was not measured in these runs.

TABLE 6 (continued).

Compound	RTI Test Number								
	16	21	23	25	33	35	36	41	43
benzene	5.0E3	-	1.4E4	6.6E3	8.1E3	6.8E3	1.1E4	1.9E4	3.4E3
toluene	3.5E4	-	5.2E3	1.0E3	3.3E3	4.0E3	3.1E3	3.0E3	2.1E3
xylenes	8.9E1	4.4E2	6.3E2	8.9E2	8.1E2	1.5E3	8.3E2	4.1E2	6.2E2
ethylbenzene	3.7E1	4.4E2	4.9E2	5.6E2	2.0E2	6.2E2	3.8E2	7.4E2	1.9E2
indan	5.9E1	2.4E1	3.4E0	7.1E0	1.4E2	3.6E1	1.4E1	7.4E1	3.7E1
indene	4.1E2	9.3E0	3.6E2	1.6E2	9.8E2	2.6E2	1.7E2	7.4E2	4.8E2
dibenzofuran	-	3.5E2	4.5E2	3.5E2	1.1E2	8.7E1	6.6E1	3.6E2	7.6E1
fluoranthene	4.0E2	7.1E2	7.1E2	3.6E2	5.8E1	2.2E1	1.4E2	1.5E3	2.3E1
fluorene	4.8E0	4.3E2	2.5E1	2.4E2	1.0E2	8.9E1	8.5E1	3.4E2	6.3E1
naphthalene	1.2E3	4.0E3	4.8E3	5.9E2	6.3E2	2.5E2	5.2E2	3.5E3	1.7E2
anthracene	7.1E2	7.7E0	4.1E2	2.0E2	1.5E2	1.4E2	2.1E2	1.0E3	1.1E2
phenanthrene	2.2E2	1.2E3	1.2E3	5.9E2	7.2E1	8.5E1	1.3E2	9.8E2	3.6E1
chrysene	-	4.3E2	4.6E2	2.4E2	3.7E1	3.6E1	4.7E1	-	9.1E1
pyrene	1.2E2	4.8E2	5.9E2	3.3E2	4.5E1	6.3E1	8.5E1	1.1E3	2.0E2
perylene	-	-	2.0E2	8.9E2	2.4E1	1.3E1	1.5E1	-	1.3E0

Note: Ammonia was not measured in these runs.

generally dominated in terms of quantity produced. Additionally, ammonia, benzene, toluene, naphthalene, and phenanthrene were present at substantial levels.

A list of selected compounds of intermediate volatility, which may easily condense from a gasifier effluent gas stream, is presented in Table 7. The quantity of each produced during gasification per unit of coal loaded into the gasifier is presented for six different tests. This table also identifies which of these compounds have been detected in products from the Morgantown fixed-bed gas producer, as well as a Chapman-Wilputte gasification unit.[5,6] Similar information for chemical compounds contained in the crude tar from various screening test runs is presented in Table 8.

Additionally, the mass of the individual fractions obtained via crude tar partitioning for the screening test runs are shown in Table 9. These values have been averaged for the various coal types utilized in order to obtain the relative amounts of individual partitions shown in Figure 2. As can be seen in this figure, the total quantity of tar generated per unit mass of coal loaded or coal converted was highest for bituminous coals, i.e., Western Kentucky No.9 and Illinois No.6, and was least for the North Dakota lignite. The Wyoming and Montana Rosebud coals were at intermediate levels relative to tar production. The PNA fraction was the predominant individual fraction in every case. While the total tar produced is very nearly the same from the gasification of Wyoming subbituminous coal and Montana Rosebud coal, the Wyoming coal resulted in larger percentage of organic acids and less PNA compounds than from the Montana coal.

The quantities of pollutants produced per unit mass of carbon converted during the coal gasification process are shown graphically in Figures 3 through 11. Numerical values are also provided representing the total amount of compound measured per unit of coal loaded into the gasifier. These bar graphs and numbers represent total pollutant quantities generated for all the various effluents collected. The compounds have been ranked so that the mass per unit of carbon converted of each of the various compounds shown may be observed. These figures represent a span of over 4 orders of magnitude in the specific pollutant mass production quantity, as expressed in units of μg pollutant per gram of carbon converted. Thus, it was necessary to represent these output values in logarithmic form in order that the specific mass values resulting could be displayed in such a comparative fashion on a single diagram.

TABLE 7. REACTOR GAS STREAMS[4,8]

Compounds produced/g coal	RTI Test No. 21	23	25	32	33	35	Found In METC Cond.	Found In METC Tar	Found In C-W Vent Gas	Found In C-W Cond.	Found In C-W Tar
Methylthiophenes	5.1E-4	4.8E-4	5.6E-6	1.0E-5	1.0E-4	3.0E-5	X				
C_2-thiophenes	2.0E-4	2.4E-4	2.5E-6	3.3E-6	2.7E-6	2.3E-5					
C_2-benzenes	2.3E-4	2.2E-4	1.4E-4	1.0E-4	≥1.1E-4	≥1.3E-5	X	X	X		
Benzofuran	5.4E-5	1.4E-4	2.5E-5	1.6E-5	NA	1.1E-4	X	X			
Indan	1.3E-5	1.5E-6	3.7E-6	4.1E-6	7.6E-5	2.0E-5	X	X			
Indene	1.2E-4	1.6E-4	7.9E-5	4.9E-5	5.4E-4	1.4E-4	X	X	X	X	X
Phenol	7.4E-5	9.9E-5	7.4E-5	1.3E-4	1.2E-3	5.9E-4	X	X	X	X	X
Cresols	1.8E-4*	2.3E-4*	2.5E-5	7.1E-5	3.2E-4	2.7E-4	X	X	X		
Xylenols	*	*	5.2E-5	1.3E-4	1.4E-3	7.0E-4			X		
Naphthalene	4.5E-4	1.5E-3	9.6E-5	2.6E-4	2.5E-4	8.5E-5	X	X	X	X	X
Biphenyl	5.0E-6	7.0E-6	1.5E-6	2.5E-6	6.3E-6	3.0E-6		X			
Diphenylmethane	8.1E-7	7.0E-6	7.4E-7	1.0E-6	2.8E-6	1.5E-6					
Dibenzofuran	2.6E-5	3.0E-5	2.2E-6	2.6E-6	1.8E-5	7.3E-6	X	X			
Anthracene	4.1E-6	3.0E-10	1.5E-6	8.1E-7	2.3E-6	1.2E-6			X		X
Phenanthrene	1.8E-6	2.0E-10	NA	NA	0	0					
C_3-benzenes	NA	NA	NA	3.9E-5	2.3E-5	1.2E-4	X	X	X		
Acenaphthene	NA	NA	NA	NA	NA	5.0E-7	X	X	X		X

C-W = Chapman-Wilputte

TABLE 8. TAR POLLUTANTS[4,8]

Compounds g produced/g coal	RTI Test Number 21	23	25	32	33	35	METC	Chapman Wilputte
Quinoline	1.0E-4	8.2E-5	5.0E-5	1.1E-5	1.0E-5	1.2E-5	NA	1.9E-3
Acridine	5.7E-5	5.0E-5	1.3E-5	3.8E-6	2.4E-6	1.1E-5	NA	9.0E-5
Naphthalene	1.9E-3	8.5E-4	2.1E-4	1.3E-4	8.9E-5	4.6E-5	7.2E-4	2.1E-4
Fluorene	2.7E-4	1.5E-4	1.3E-4	4.6E-5	5.7E-5	4.8E-5	1.6E-5	2.4E-4
Dibenzofuran	2.5E-4	1.7E-4	9.4E-5	3.8E-5	4.1E-5	4.2E-5	1.5E-4	NA
Fluoranthene	4.1E-4	4.3E-4	1.9E-4	1.4E-4	3.2E-5	1.2E-5	NA	1.4E-4
Chrysene	2.7E-4	2.8E-4	1.3E-4	9.7E-5	2.1E-5	7.0E-6	NA	2.9E-4
Perylene	NA	1.2E-4	4.7E-5	7.4E-5	1.3E-5	7.5E-5	NA	8.0E-5
Anthracene	NA	2.4E-4	1.1E-4	1.5E-4	8.2E-5	7.5E-5	NA	6.E3-4
Phenol	9.7E-5	1.5E-4	7.5E-5	3.8E-5	1.6E-4	3.3E-4	1.4E-5	1.8E-4
Cresols	3.7E-4	4.6E-4	1.3E-4	1.2E-4	3.5E-4	7.7E-4	6.0E-4	NA

*Maximum of three samples assumed 0.034 g tar/g coal.

TABLE 9. WEIGHT PERCENT OF INDIVIDUAL FACTIONS OBTAINED FROM CRUDE TAR PARTITIONING

	Test Number							
	6	16	20	21	23	25	26	32
Tar Mass (grams)	15.9	56.5	54.3	5.11	52.33	26.42	26.46	14.7
% Organic Acids	30.3	13.2	13.96	10.05	12.9	11.1	13.3	14.6
% Organic Bases	12.5	6.0	5.52	7.49	7.2	4.8	6.6	5.3
% Insoubles	13.9	9.5	16.70	10.15	11.3	2.8	5.4	6.2
% Nonpolar Neutrals	13.0	29.8	12.56	13.95	11.1	7.4	17.2	16.5
& PNA's	16.5	33.3	44.49	53.13	53.6	68.7	51.4	51.9
% Polar Neutrals	13.8	8.1	6.76	5.23	4.0	5.2	6.0	5.5
% Tar/Coal	1.54	3.59	3.44	3.30	3.26	1.77	1.78	1.081

	Test Number							
	33	35	36	38P	38G	41	43	44
Tar Mass (grams)	16.823	41.2	12.0	1.194	12.93	37.56	10.49	30
% Organic Acis	26.9	29.6	--	9.93	20.37	5.22	25.28	6.47
% Organic Bases	3.3	3.4	--	1.04	3.73	7.06	5.42	6.49
% Insolubles	1.7	4.1	--	1.82	0.33	8.05	5.66	4.80
% Nonpolar Neutrals	20.4	18.3	--	49.68	23.75	12.50	20.70	11.22
% DNA's	39.8	35.4	--	29.94	35.57	61.75	33.21	67.38
% Polar Neutrals	7.8	9.2	--	7.59	11.45	5.42	9.73	3.64
% Tar/Coal	1.20	2.90	--	0.159	1.72	3.00	0.719	2.40

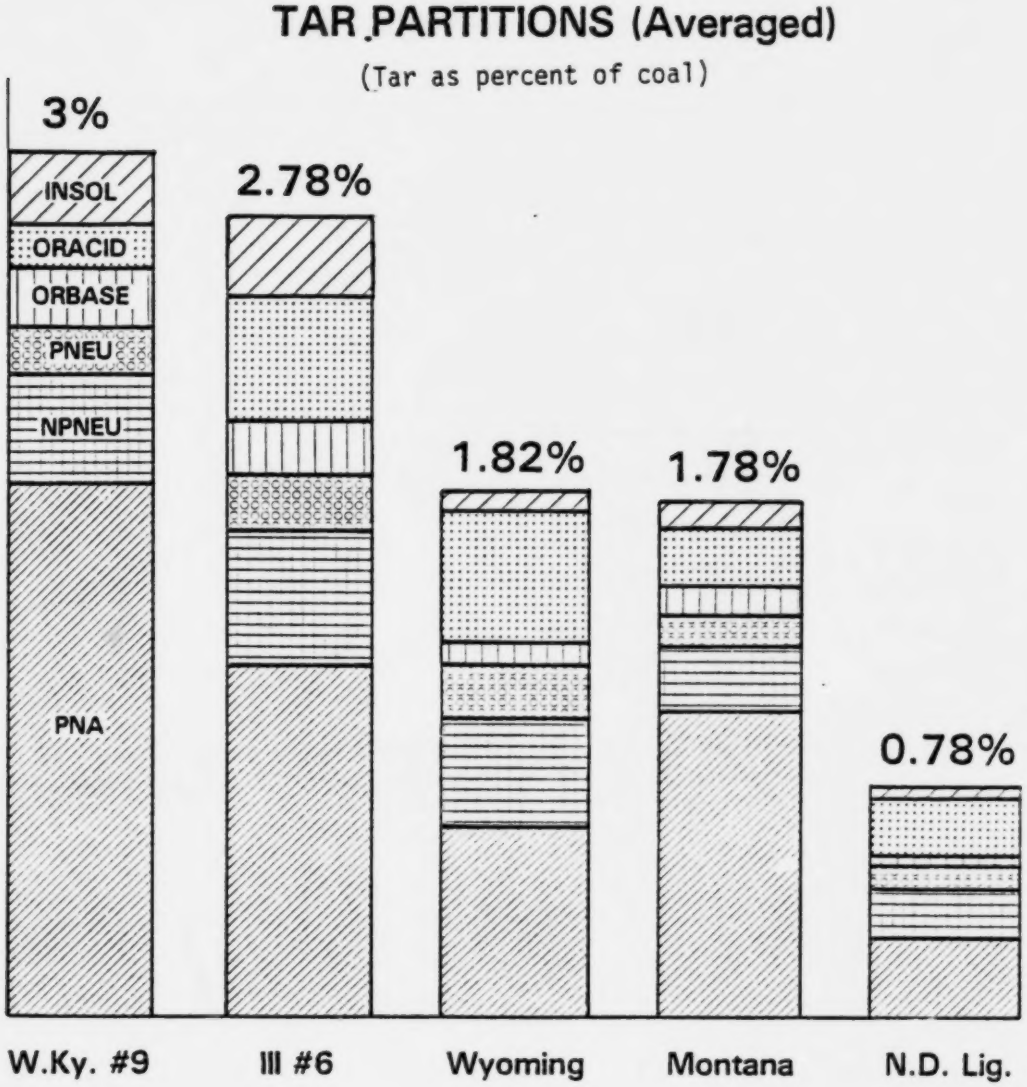

Figure 2. Tar partitions.

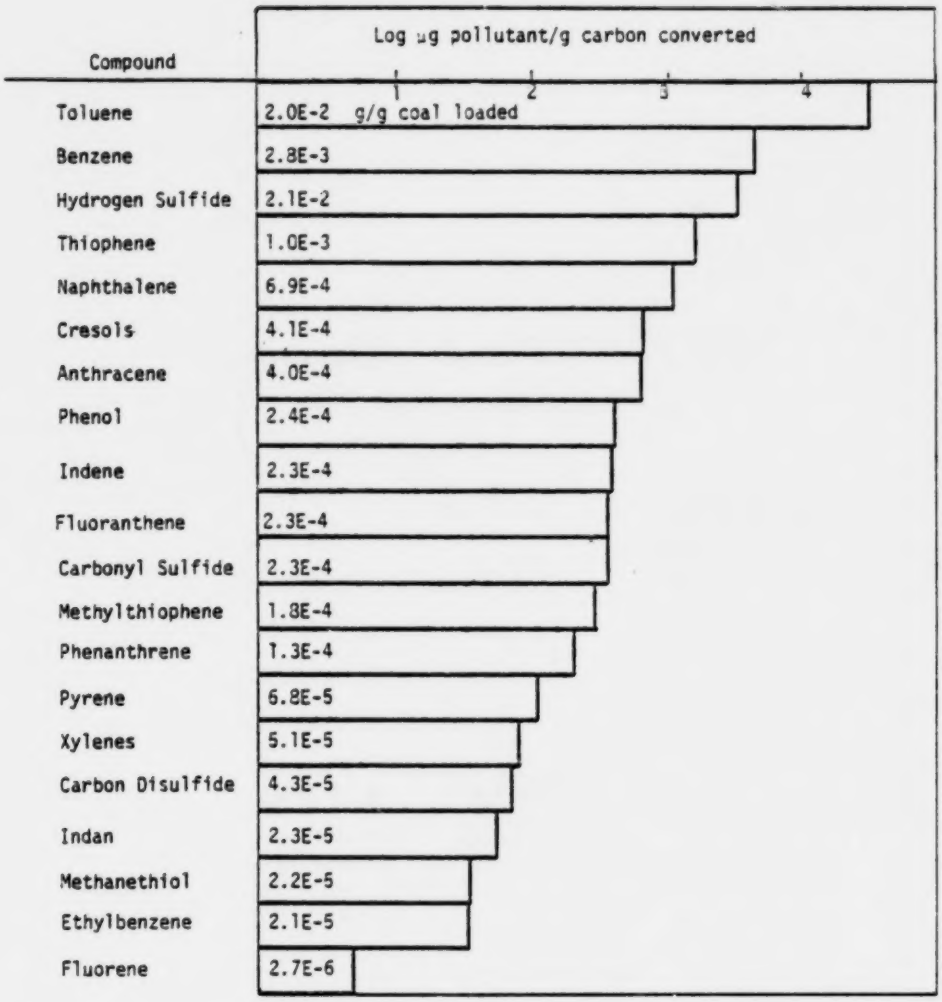

Figure 3. Production factors for major pollutants from run no. 16 with Illinois No.6 coal. NOTE: Ammonia was not measured in this run.

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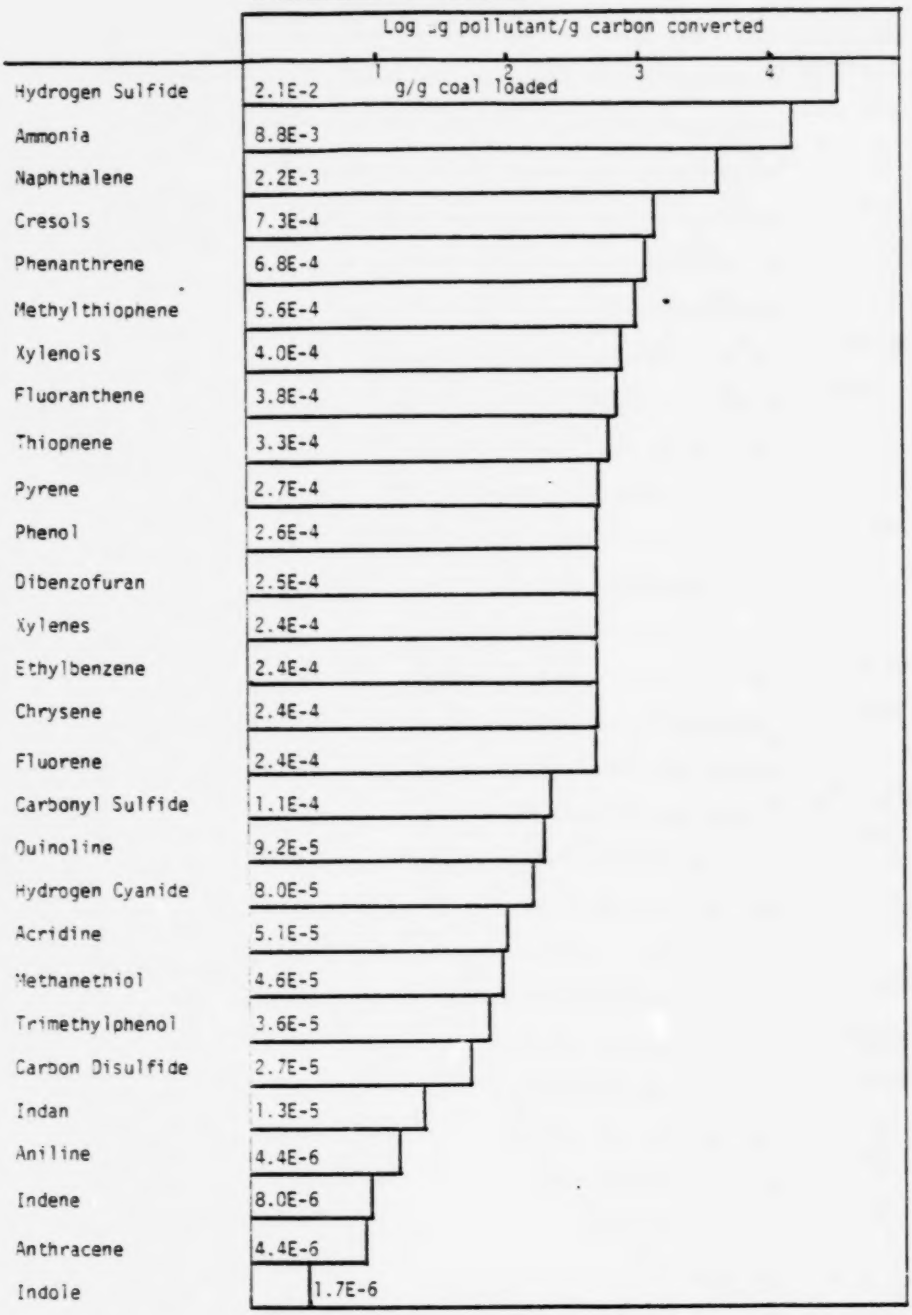

Figure 4. Production factors for major pollutants from run no. 21 with Illinois No.6 coal.

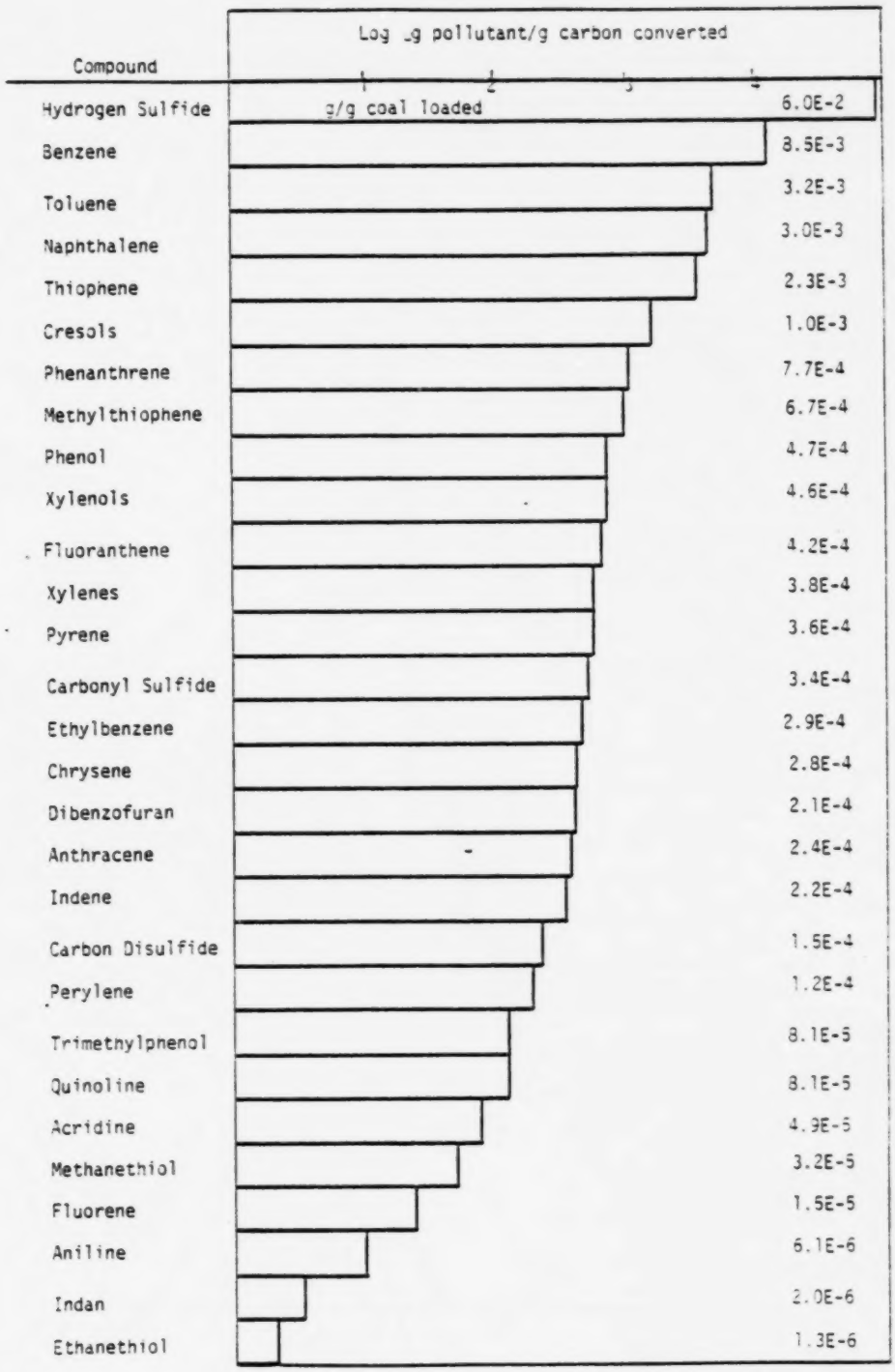

Figure 5. Production factors for major pollutants from run no. 23 with Illinois No.6 coal. NOTE: Ammonia was not measured in this run.

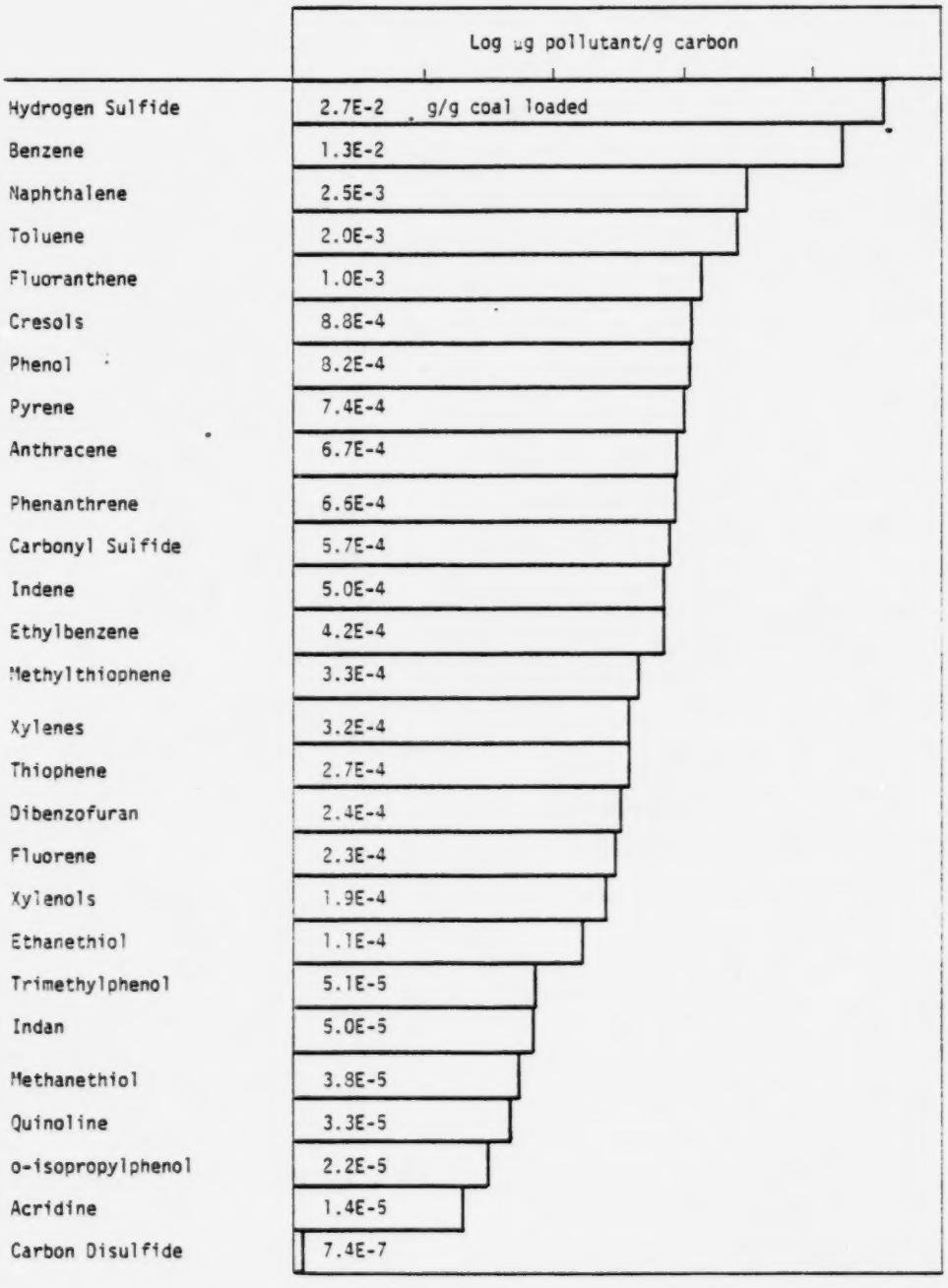

Figure 6. Production factors in major pollutants from run no.41 with Western Kentucky No.9 coal. NOTE: Ammonia was not measured in this run.

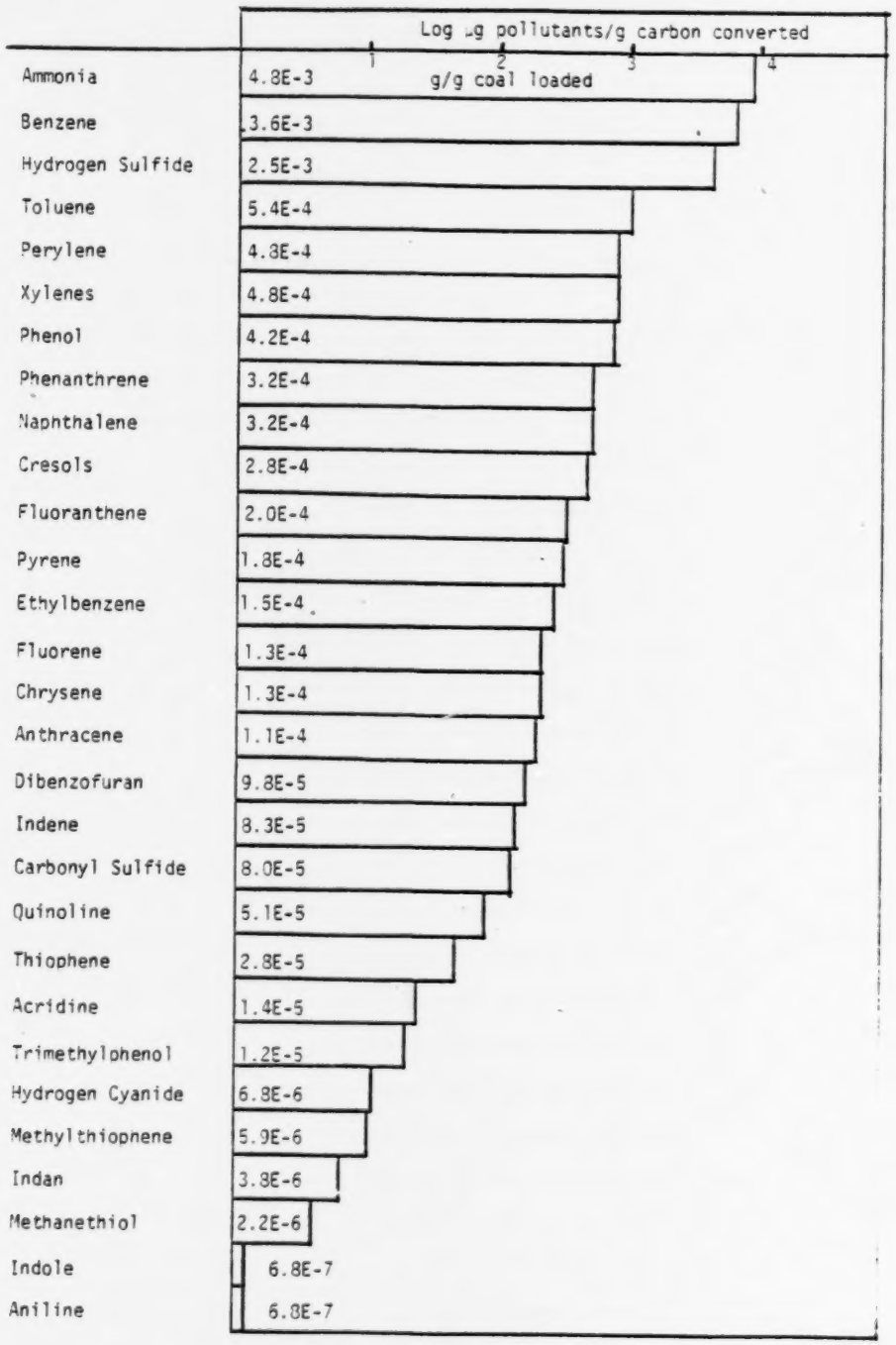

Figure 7. Production factors for major pollutants from run no.25 with Montana Rosebud coal.

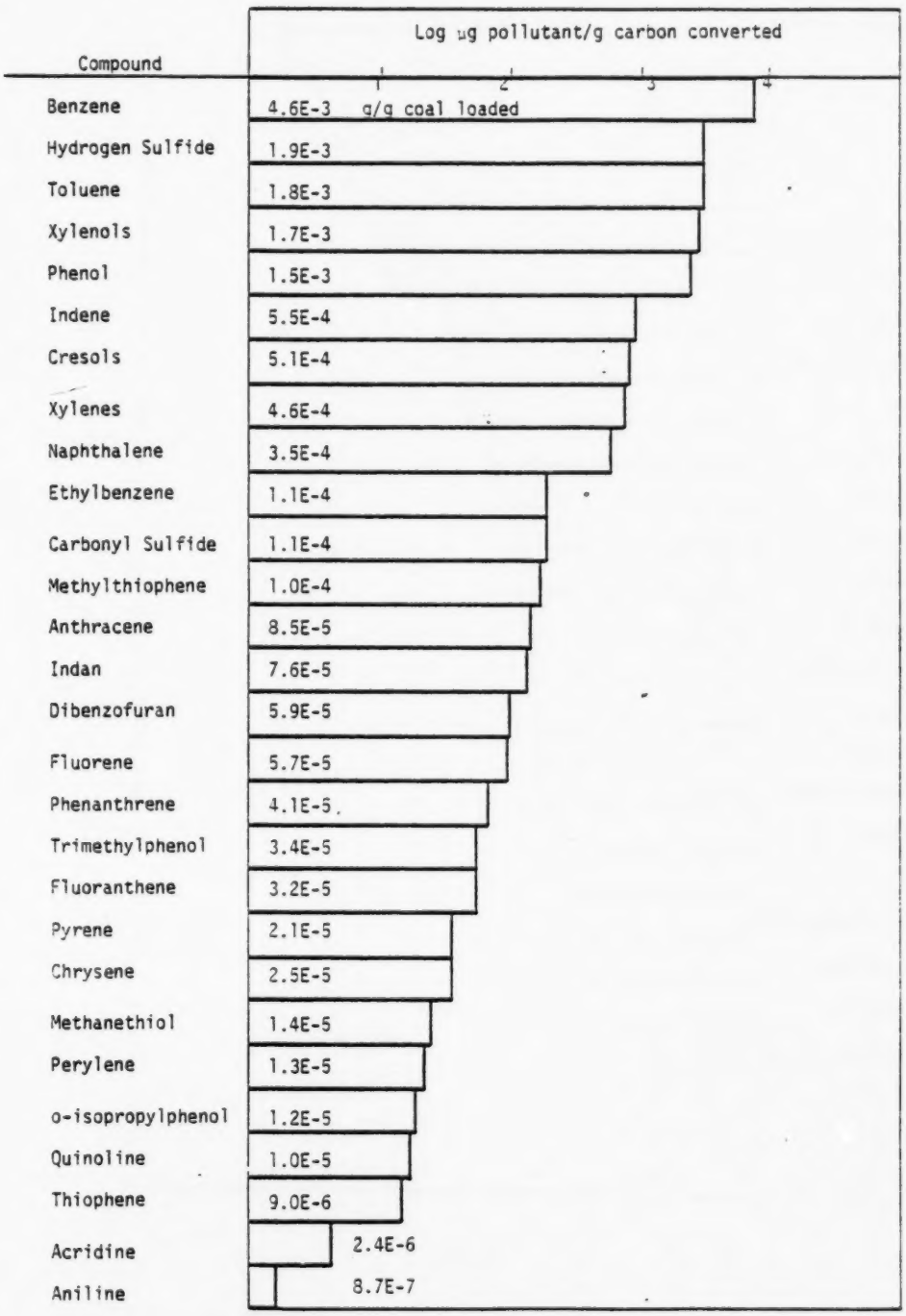

Figure 8. Production factors for major pollutants from run no.33 with Wyoming subbituminous coal. NOTE: Ammonia was not measured in this run.

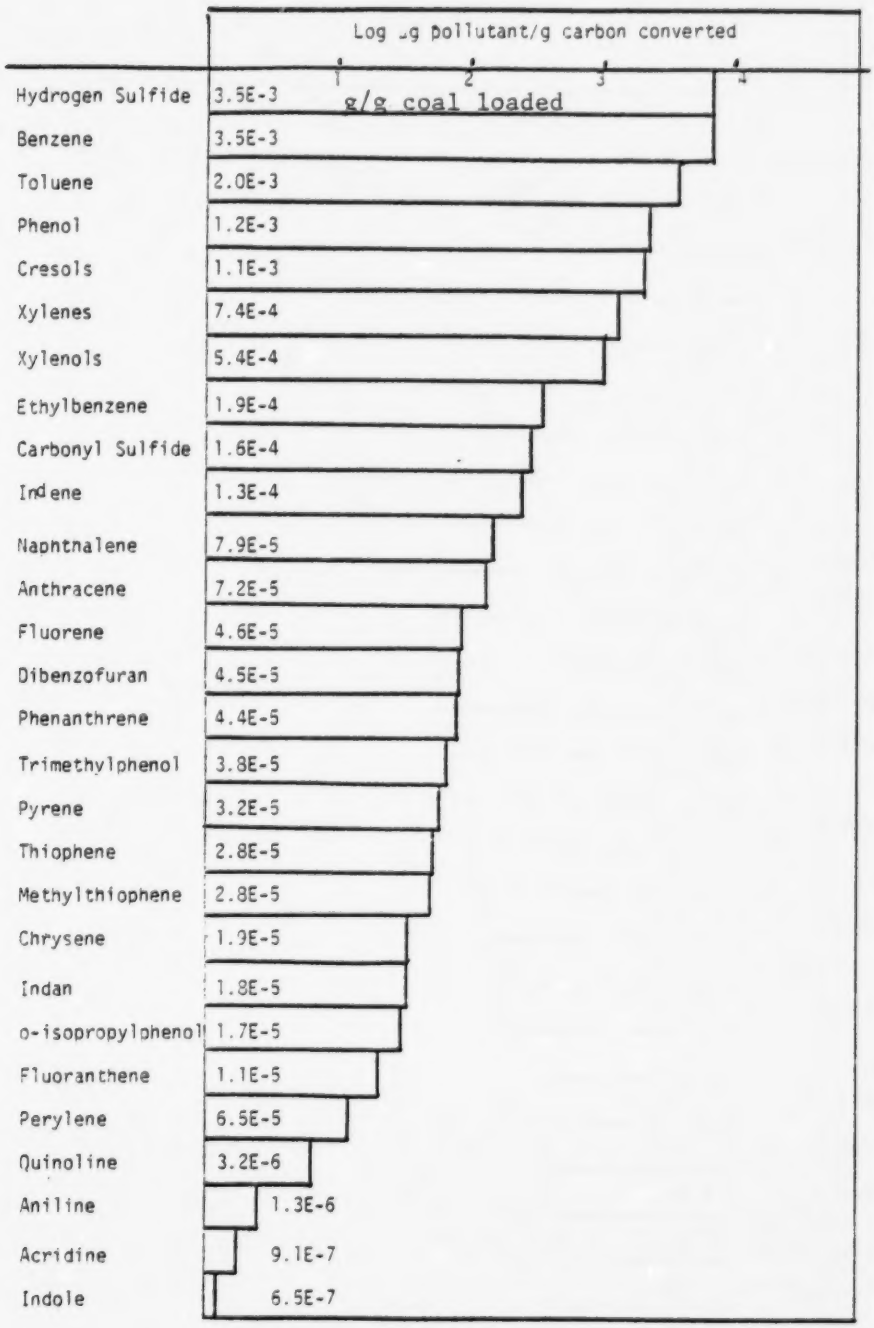

Figure 9. Production factors for major pollutants from run no. 35 with Wyoming subbituminous coal. NOTE: Ammonia was not measured in this run.

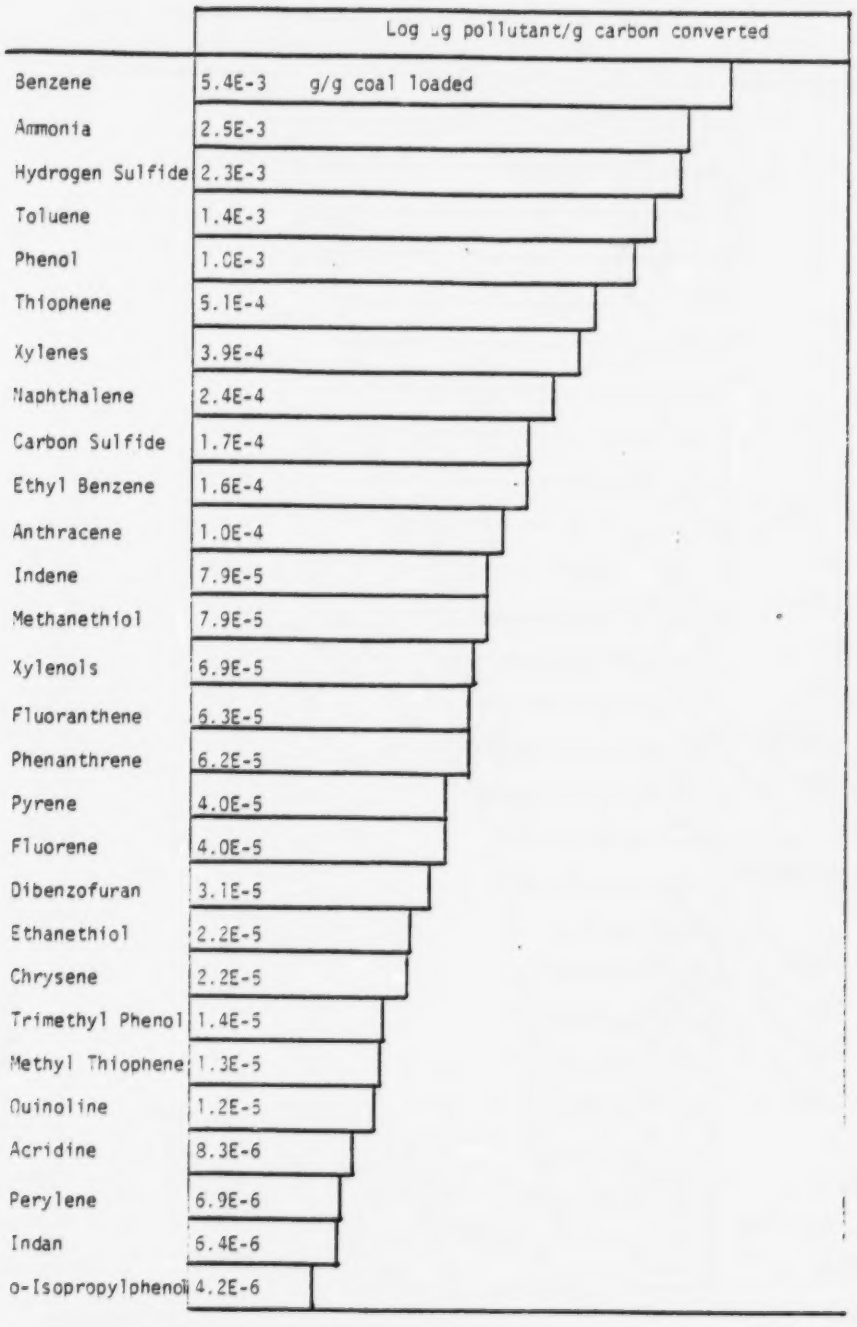

Figure 10. Production factors for major pollutants from run no. 36 with North Dakota Zap lignite coal.

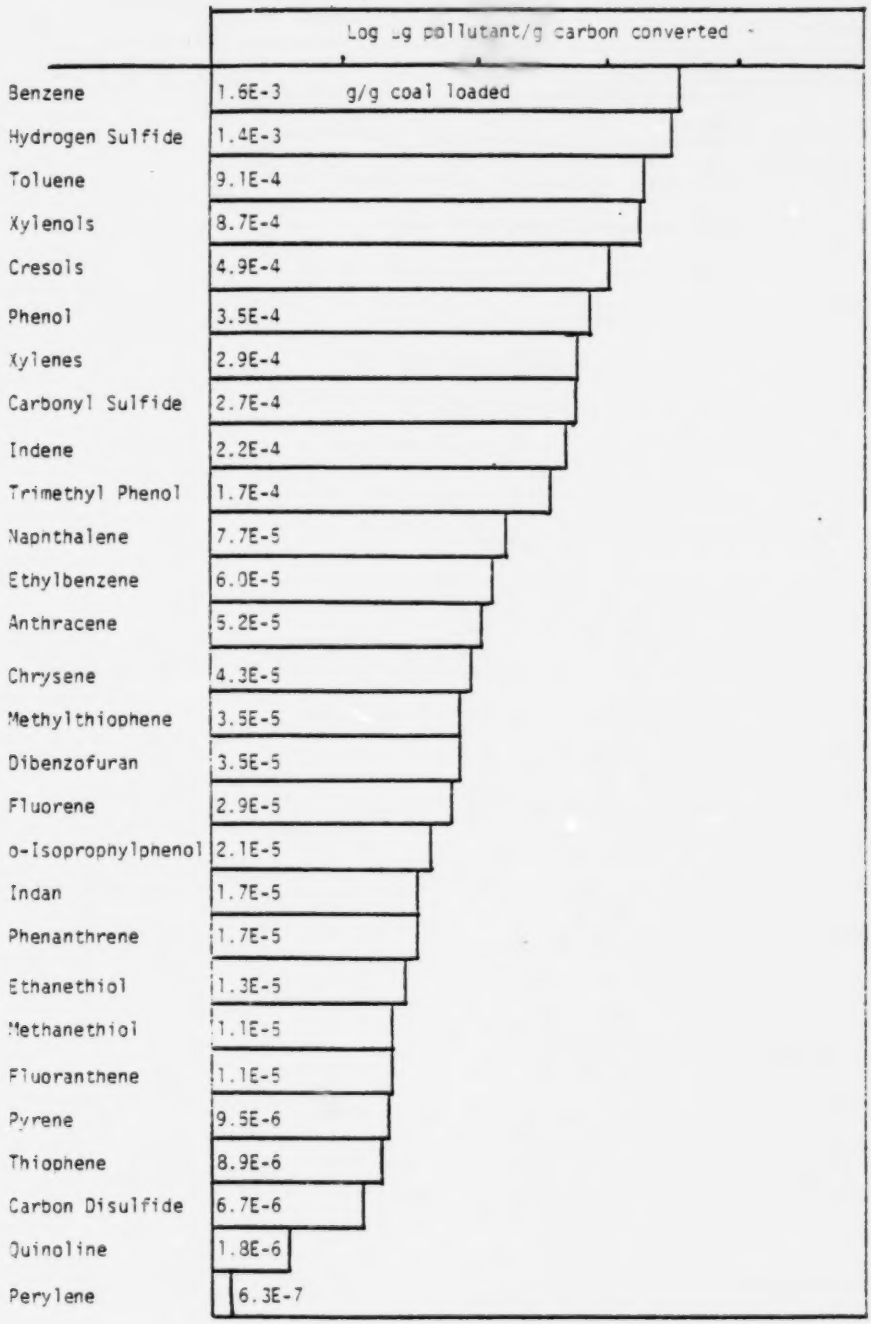

Figure 11. Production factors for major pollutants from run no. 43 with North Dakota Zap lignite coal. NOTE: Ammonia was not measured in this run.

Figures 3 through 11 indicate that no consistent hierarchy of compounds exists regardless of whether one considers compounds produced from an individual coal or from coals of equal rank gasified under alternative operating conditions. Ammonia was not measured in all of these tests; yet, it is known that ammonia occurs at high levels in the effluent of gasifiers operating on fuels containing nitrogen. It is important to note that benzene, toluene, and xylene as well as sulfur species, phenolic compounds, and two-ring PNAs were important in every case.

The composition of the major elements in selected tars (low volatile organic condensate) is shown in Table 10. While the sulfur and nitrogen content of these materials is relatively high, the higher oxygen content indicates that phenolic, carboxylic, and other hetero-oxygen compounds are present in relatively significant quantities.

In order to effectively analyze the extensive data obtained during the screening test sequence, material balance computations and statistical correlation analyses were performed. Data values were entered into a computer memory for the statistical analysis. Stepwise multiple linear regression techniques were utilized in order to effectively evaluate the influence of the independent variables present during these experiments. The material balance results, as well as the statistical analysis technique and results, are discussed in the following sections.

TABLE 10. PRIMARY ELEMENTS OF TARS[1,4,9]

Run No.	Coal Type	Weight Percent of Element in Tar				
		% Carbon	% Hydrogen	% Nitrogen	% Sulfur	% Oxygen
6	Illinois No.6	78.7	6.3	1.3	2.9	10.9
15	Illinois No.6	87.5	6.1	1.3	1.9	3.2
16	Illinois No.6	87.6	6.2	2.1	1.6	2.4
21	Illinois No.6	87.7	6.1	1.4	1.8	3.1
23	Illinois No.6	86.0	5.8	1.6	2.5	3.8
25	Montana Rosebud	88.6	6.0	0.8	0.7	4.0
33	Wyoming Subbituminous	86.5	6.0	0.8	2.4	4.3
35	Wyoming Subbituminous	83.0	7.7	1.5	0.5	7.4
36	North Dakota Lignite	86.1	7.0	1.3	0.7	4.9
41	Western Kentucky No.9	86.3	6.1	1.6	2.7	2.8
43	North Dakota Lignite	82.3	7.5	1.8	0.9	7.0
METC	Montana Rosebud	78.0	6.6	1.1	2.4	11.0
METC	Western Kentucky No.9	80.0	8.7	1.9	2.7	NA
METC	New Mexico Subbituminous	84.4	7.2	1.7	1.4	NA

4.0 MATERIAL BALANCE RESULTS

A variety of screening tests have been performed in the RTI fixed-bed gasifier. One purpose of these tests was to develop operating procedures and sampling techniques for the gasifier. Nine runs representing five coal types were chosen as candidates for complete material balances on ash and the major elements: hydrogen, oxygen, carbon, nitrogen and sulfur. The material balances were taken over the length of the gasification run which was considered to be the time from the coal drop to oxygen breakthrough.

Results of the material balances are summarized in Table 11. It can be seen that the average of the overall material balance for each of the runs gives a 100 percent closure but with a standard deviation of 13 percent. The other component balances except sulfur are within 11 percent of closure but they also have a large standard deviation indicating considerable scattering of the closures. Sulfur is the component in the material balances which appears in the smallest amounts. The deficiency in the closure of the sulfur balances is probably due to the sampling procedure used in these preliminary screening runs. This point as well as experimental deviations in other balances are discussed in more detail below. Also discussed is the possible improvement of the balances obtained by making judicious and reasonable changes in experimental values that could perhaps be in error.

4.1 COMPUTATION PROCEDURE

Detailed material balances were performed for various runs on each of the five coals considered. The amount of each of the major components in the various inlet or outlet streams was computed. Sample results are shown in Tables 12 through 16.

The coal charge for each experiment was measured within ± 1 gram using a scale; however, it was found that 4 to 5 grams of coal usually retained in the coal feeder giving an error of up to 0.5 percent in the coal feed reported in Tables 12 through 16. An ultimate analysis of the coal charges for each individual run was not made and this could be a source of considerable error due to changes in moisture content. The amount of each major element in the

TABLE 11. ELEMENTAL BALANCES FOR RTI SCREENING RUNS
% Closure (outlet wt./inlet wt.)

RUN #	OVERALL	HYDROGEN	OXYGEN	CARBON	NITROGEN	SULFUR	ASH
16	74 (96)	64 (99)	64 (100)	81	94	75	114
21	91 (97)	86 (95)	91 (100)	86	96	63	123
23	117 (100)	114 (100)	119 (100)	97	121 (99)	114	118
25	97	82	101	86	100	72	85
33	98	100	104	84	100	53	65
35	107 (100)	80 (98)	92 (99)	91 (100)	126 (100)	12	107
36	99 (101)	80 (112)	90 (100)	87 (100)	115 (104)	48	74
41	106 (100)	118 (109)	109 (100)	106	105 (100)	81	72
43	111 (101)	95 (115)	105 (100)	87 (100)	128 (101)	73	123
Standard Deviation	13 (2)	17 (10)	16 (1)	8 (9)	13 (3)	28[20]*	24

[ ]* Excludes Run #35

NOTE: By adjusting selected experimental values, results shown in parentheses are obtained.

TABLE 12. MATERIAL BALANCE RESULTS FOR RUN NO.16 (ILLINOIS NO.6 BITUMINOUS COAL)

Component	Total Amount*	Hydrogen Amount	Oxygen Amount	Carbon Amount	Nitrogen Amount	Sulfur Amount	Ash Amount
Coal	1572.8	83.36	191.88	1046.54	23.91	48.44	178.67
Steam	4110.0	456.67	3653.33	-	-	-	-
Air	2021.4	-	380.76	-	1640.60	-	-
Total Input	7704.2	540.03	4225.97	1046.54	1664.51	48.44	178.67
Gas	3569.2	147.78	1147.59	680.32	1561.53	31.97	-
Condensate	1734.0	192.67	1541.33	-	-	-	-
	(3461.6)	(384.62)	(3076.95)	-	-	-	-
Tar	59.6	3.69	1.43	52.25	1.24	0.95	-
Residue	325.7	0.94	0.00	115.85	1.04	3.42	204.44
Total Output	5688.5	345.08	2690.35	848.42	1563.61	36.34	204.44
	(7416.1)	(537.03)	(4225.97)	-	-	-	-
Balance, %	74	64	64	81	94	75	114
	(96)	(99)	(100)	-	-	-	-

*Amounts in Grams

NOTE: By adjusting selected experimental values, results shown in parentheses are obtained.

TABLE 13. MATERIAL BALANCE RESULTS FOR RUN NO.25 (MONTANA SUBBITUMINOUS COAL)

Component	Total Amount *	Hydrogen Amount	Oxygen Amount	Carbon Amount	Nitrogen Amount	Sulfur Amount	Ash Amount
Coal	1495.0	102.71	426.52	806.55	17.94	8.82	132.46
Steam	704.0	78.22	625.78	-	-	-	-
Air	2901.1	-	676.00	-	2225.13	-	-
Total Input	5100.1	180.93	1728.30	806.55	2243.07	8.82	132.46
Gas	4020.9	60.82	1051.49	673.04	2232.23	3.30	-
Condensate	783.0	87.00	696.00	-	-	-	-
Tar	24.4	-	-	22.78	-	1.64	-
Residue	114.3	0.23	0.12	0.46	0.11	1.37	112.0
Total Output	4942.6	148.05	1747.61	696.28	2232.34	6.31	112.0
Balance, %	97	82	101	86	100	72	85

*Amounts in Grams

TABLE 14. MATERIAL BALANCE RESULTS FOR RUN NO.33 (WYOMING SUBBITUMINOUS COAL)

Component	Total Amount*	Hydrogen Amount	Oxygen Amount	Carbon Amount	Nitrogen Amount	Sulfur Amount	Ash Amount
Coal	1399.6	83.14	420.16	793.57	5.32	9.10	88.31
Steam	504.0	56.00	448.00	-	-	-	-
Air	2027.7	-	472.45	-	1555.25	-	-
Total Input	3931.3	139.14	1340.61	793.57	1560.57	9.10	88.31
Gas	3219.2	75.43	905.30	651.49	1584.27	2.72	-
Condensate	545.0	60.56	484.44	-	-	-	-
Tar	16.8	1.86	5.37	7.61	0.73	1.25	-
Residue	71.4	0.87	1.36	11.20	0.10	0.88	57.0
Total Output	3852.4	138.72	1396.47	670.30	1585.10	4.85	57.0
Balance, %	98	100	104	84	100	53	65

*Amounts in Grams

TABLE 15. MATERIAL BALANCE RESULTS FOR RUN NO.36 (NORTH DAKOTA LIGNITE COAL)

Component	Total Amount*	Hydrogen Amount	Oxygen Amount	Carbon Amount	Nitrogen Amount	Sulfur Amount	Ash Amount
Coal	1446.7	94.90	563.63	677.04	10.56	8.10	92.44
Steam	629.8	69.98	559.82	-	-	-	-
Air	2414.4	-	562.57	-	1851.79	-	-
Total Input	4490.9	164.88	1686.02	677.04	1862.35	8.10	92.44
Gas	3681.2	56.23	910.16	572.65	2139.23	2.94	-
	(3590.6)	(86.44)	-	(663.29)	(1927.74)	-	-
Condensate	676.0	75.11	600.89	-	-	-	-
	(871.1)	(96.79)	(774.30)	-	-	-	-
Tar	14.9	1.15	1.25	12.17	0.13	0.16	-
Residue Particulates	71.6	0.11	0.31	1.88	0.04	0.77	68.44
Total Output	4443.7	132.60	1512.61	586.70	2139.40	3.87	68.44
	(4548.2)	(184.49)	(1686.02)	(677.34)	(1927.91)	-	-
Balance, %	99	80	90	87	115	48	74
	(101)	(112)	(100)	(100)	(104)	-	-

*Amounts in Grams

NOTE: By adjusting selected experimental values, results shown in parentheses are obtained.

TABLE 16. MATERIAL BALANCE RESULTS FOR RUN NO.41 (WESTERN KENTUCKY BITUMINOUS COAL)

Component	Total Amount*	Hydrogen Amount	Oxygen Amount	Carbon Amount	Nitrogen Amount	Sulfur Amount	Ash Amount
Coal	1250.0	62.37	230.54	786.59	17.39	37.14	115.63
Steam	1388.0	154.22	1233.78	-	-	-	-
Air	3764.2	-	877.06	-	2887.16	-	-
	(3956.2)	-	(921.80)	-	(3034.44)	-	-
Total Input	6402.0	216.59	2341.38	786.59	2904.55	37.14	115.63
	(6594.2)		(2386.12)		(3051.83)		
Gas	5316.4	101.48	1334.36	800.56	3050.96	28.99	-
Condensate	1360.0	151.09	1208.75	-	0.16	-	-
	(1183.3)	(131.46)	(1051.67)	-	-	-	-
Tar	35.0	3.27	-	30.05	0.71	1.01	-
Residue Particulates	84.0	0.01	0.09	0.04	-	0.02	83.80
Total Output	6795.4	255.85	2543.20	830.65	3051.83	30.02	83.80
	(6618.7)	(236.22)	(2386.12)				
Balance, %	106	118	109	106	105	81	72
	(100)	(109)	(100)		(100)		

*Amounts in Grams

NOTE: By adjusting selected experimental values, results shown in parentheses are obtained.

coal feed was obtained by multiplying the coal charge by the as-received ultimate analysis.

Steam was fed to the gasifier at a constant rate using a positive displacement metering pump. The accuracy of the steam input is thought to be fairly high, i.e., ± 5 percent, since the pump was calibrated prior to use.

The flow of air to the gasifier was not constant since it was used to maintain the maximum temperature in the gasifier below a specified limit. The flow rate measurement was based on the heat capacity of the gas and could have been in error by 10 percent. The total flow of air was obtained by integrating the flow measurements taken at least every two minutes over the length of the run.

The flow of product gas was estimated by differentiating the dry test meter data; from a consideration of system leakage, flow rate was estimated to be accurate to within ± 20 percent. The composition of the gases were determined by two independent measurements. The gas composition was monitored every two minutes for CO, CO_2, CH_4, and H_2. The accuracy of these measurements of CO, CO_2, and CH_4 was considered to be within ± 1 percent of the measured percentage but the H_2 measurement could be in error by as much as ± 3 percent. Bulb samples were taken throughout the runs. These were analyzed for the major components as well as minor components such as benzene, toluene, xylene, and sulfur compounds. Major gases were detected within a 2 percent accuracy, and BTX and sulfur compound measurements were estimated to be accurate within 10 percent. In order to perform material balances on the gasification runs shown in Tables 12 through 16, the discrete concentration values were multiplied by the flow rate and summed (integrated) over the duration of the run. The integrated data showed that up to 8 percent of the product gas was unaccounted for in these data. Sources of error in the integration could be due to inaccurate flow rates and/or inaccurate measurement of the time intervals between samples. In coal gasification the devolatilization of coal takes place rapidly; thus, if only a few sample bulbs are taken during the initial stage of a batch run, considerable amounts of devolatilization products may leave the system undetected. This could explain the nonclosure of the sulfur balances shown in Table 11.

The condensate is measured volumetrically and this measure is converted to weight. The accuracy in the measurement is estimated to be normally within

± 5 percent. In cases where the condensate was analyzed for contaminants, the contaminants were considered in the elemental breakdown of the condensate. Otherwise, the condensate was considered to be essentially water.

The amounts of tar reported in Tables 12 through 16 consist of the actual tar phase plus organics extracted from the condensate. The ultimate analysis of the tar was determined by standard techniques. In several runs the tar analyses were not available and the composition of the tar was estimated from the analysis of tars from runs using the same coal. This procedure could introduce little error into the elemental balances because of the small amounts involved.

The residue is weighed accurately; however, there are inadvertent losses in removing the residue from the gasifier. The ultimate analysis was obtained by standard procedures. The weight of particulates retained in the filter in most cases was not taken. Several of the runs showed a net loss of ash. The missing ash could be contained in the unmeasured particulates.

4.2 MATERIAL BALANCE ADJUSTMENTS

Better closures of the material balances can be obtained by the reasonable adjustment of selected experimental measures. For example, in Table 12 it can be seen that 4110 g of steam was fed to the gasifier but that only 1734 g of condensate is reported to be collected. This represents a steam conversion of 58 percent which is not typical for Illinois No. 6 coal. By increasing the condensate mass so that the oxygen closure is assured, the hydrogen and overall balances approach 100 percent closure for the run, as can be seen in Table 12. In Table 16 both the air flow and condensate measurements were adjusted to ensure closure of nitrogen and oxygen. This resulted in improvements to both the overall balance and the hydrogen balance.

Table 15 shows a case where both the condensate and gas analysis were adjusted to give closure of carbon and oxygen resulting in improved closures of the hydrogen and nitrogen balances. The corrected amount of condensate shown in Table 15 appears too large, in that it exceeds the steam input; however, taking into account the moisture in the lignite coal, the corrected condensate corresponds to almost 20 percent steam decomposition.

Adjustments similar to those discussed above were made in several other runs. Table 11 summarizes these results. It can be seen that the average of

the closures for each of the major components is improved and that the scatter within the closures is reduced. Some of the arbitrariness involved in the adjustments could be removed from the material balance analyses using a well-known procedure which minimizes the sum of the weighted squares of the differences between an experimental measurement and a computed measurement, where the computed composition analysis must sum to 1.0. There is sufficient redundancy of measurements in the RTI gasifier system that this procedure could be used. Such may be justified for the parametric test runs, for which more precise control is being exercised over the reaction process.

The adjusted material balances for the nine gasifier runs as summarized in Table 11 demonstrate that the major elements can, in principle, be accounted for in semibatch experiments. RTI is presently attempting to further reduce the errors in the material balances by performing gas bulb sampling more frequently in the initial stage of the runs, and using improved operating procedures and calibration techniques.

4.3 TRACE ELEMENT BALANCES

Samples of aqueous condensate, tars, and reactor residues were subjected to atomic absorption measurement so as to determine the levels of various trace elements present. Table 17 presents the results of tar and condensate analysis for antimony, arsenic, cadmium, and lead. Arsenic, beryllium, cadmium, lead, mercury, and selenium analyses were determined in the reactor residue samples as shown in Table 18. These tables present trace element concentrations in μg/g for the gasifier effluents as well as the percentage of the element originally present in the feed which was recovered in the tar, condensate and gasifier ash. The operating conditions for each run shown are presented in Table 3.

The trace element behavior is seen in these tables to be quite variable. Two important factors may be primarily responsible. First the feed coals varied greatly in their inherent trace element contents. Then, individual coal charges were not always analyzed separately, allowing possible error due to non-homogeneity within a given coal type. Further, the metallic elements present in the reactor system, viz., iron, nickel, cadmium, and manganese, may have entered various of the samples as a result of corrosion phenomena.

TABLE 17. TRACE METAL ANALYSES (TAR AND CONDENSATE)
µg/g (% Recovered)

TEST	16	21	23	25	33	35	36
			Tar µg/g (% Recovered)				
Antimony	NA	NA	NA	NA	0.14(0.3)	.095(5.4)	.42(2.6)
Arsenic	1.3(1.4)	4.2(4.3)	4.6(4.7)	NA	.20(0.3)	.48(1.9)	.66(0.2)
Cadmium	NA	.035(1.7)	.027(0.8)	NA	NA	.017(1.9)	.042(0.6)
Lead	NA	1.1(1.5)	.31(0.4)	NA	NA	.73(21)	2.1(6.8)
			Condensate µg/ml (% Recovered)				
Antimony	0.014(26)	0.0035(13)	0.0096(23)	<.003	<.003	<.003	<.003
Arsenic	0.0063(2.3)	0.23(16)	0.44(20)	0.11(4.6)	0.036(2.0)	0.013(0.7)	0.029(0.6)
Cadmium	NA	0.0038(12)	0.00013(0.2)	0.0044(3.4)	NA	0.015(22)	0.00013(0.1)
Lead	NA	0.030(2.8)	0.012(0.7)	0.0085(0.7)	NA	0.021(7.8)	0.044(9.0)

NA = Not Analyzed

No Tar or Condensate Analyses Available for Tests 41 or 43

TABLE 18. TRACE METAL ANALYSES - RESIDUE (BOTTOM ASH)
µg/g (% Recovered)

TEST	16	21	23	41	25	33	35	36	43
Arsenic	13(84)	12(51)	9.1(46)	7.2(20)	4.8(29)	16(90)	8.3(77)	41(84)	54(112)
Beryllium	NA	6.5(99)	4.5(82)	11(100)	4.9(95)	NA	3.4(67)	3.7(52)	3.2(46)
Cadmium	NA	0.88(177)	0.41(108)	1.8(188)	0.028(3.1)	NA	0.22(57)	0.51(43)	1.0(87)
Lead	NA	9.0(54)	4.9(34)	NA	2.1(27)	NA	2.3(154)	1.4(28)	0.53(11)
Mercury	<1	<1	<1	NA	<1	NA	<1	NA	NA
Selenium	3.0(41)	1.4(13)	1.7(18)	9.9(30)	1.8(18)	NA	5.9(37)	NA	15(104)

NA = Not Analyzed

Beryllium was presented at low levels in the coals and was retained principally in the reactor residue. Beryllium retention was most pronounced for the higher rank coals. Arsenic retention was higher for the lower rank coals. Cadmium levels indicate that contamination from the metallic reactor system may have taken place. The unusually low recovery for cadmium in Run 25 (Montana Rosebud) as compared with the other coals studied (3.1 percent versus 43 percent or higher) may be due to the use of a nonrepresentative coal sample for the original trace element determination. (Trace element determinations for parametric runs are being performed by selecting samples for analysis from small aliquots which have been specifically prepared for each run.)

A comparison of selected trace element distribution results of the RTI screening tests with those available from various research gasifiers are presented in Table 19. The RTI gasifier was found to accumulate arsenic in the reactor residue when gasifying Pittsburgh No.8 seam coal, as shown in Table 19. This may be an error or artifact, rather than an actual condition. The Synthane PDU gasifier of the Pittsburgh Energy Technology Center was found to accumulate arsenic, cadmium and lead when operating with an Illinois No.6 coal. This may be associated with the fact that the Synthane gasification process does not achieve a high carbon conversion as a result of limited fluidized bed residence time. (The resulting char material is assumed to be useful in alternative conversion steps in order to fully utilize the carbon content of the material.)

Overall, the comparative data indicate that trace element behavior is quite variable in gasification processes. Low elemental recovery rates indicate that significant percentages of the elements escape to one or more effluents. Arsenic, cadmium, lead, and mercury must then all be regarded as potentially volatile elements in coal gasification reactors.

Table 19. COMPARISON OF TRACE ELEMENT ANALYSIS RESULTS [10,11,12]

Mass Fraction (µg/g)	Arsenic		Cadmium		Lead		Mercury	
Feed Process Research Group	Feed	Residue	Feed	Residue	Feed	Residue	Feed	Residue
Pittsburgh No. 8 Coal RTI Gasifier Research Triangle Institute	8.71	20.6	0.16	0.01	6.50	2.62.	0.13	<0.03
Pittsburgh No. 8 Coal Hygas PDU Gasifier Institute of Gas Technology	9.6	3.4	0.78	0.30	5.9	2.2	0.27	0.01
Illinois No. 6 Coal RTI Gasifier Research Triangle Institute	3.26	2.39	0.34	0.13	16.8	0.30	0.12	<0.03
Illinois No. 6 Coal Hygas PDU Gasifier Institute of Gas Technology	24	16	0.89	0.21	11	5.8	0.12	<0.01
Illinois No. 6 Coal Synthane PDU Gasifier Pittsburgh Energy Research Center	1.3	3.3	0.01	0.77	1.1	21	0.14	ND
Montana Rosebud Coal RTI Gasifier Research Triangle Institute	0.71	<0.02	0.14	0.04	20.5	1.98	0.10	<0.03
Montana Rosebud Coal GEGAS Gasifier Peabody Coal Company	2.6	1.2	1.0	6.1	1	51	0.09	0.12

ND = Not detected.

5.0 STATISTICAL ANALYSIS OF DATA

A statistical analysis of the RTI gasifier screening runs was carried out to identify the most important operating parameters affecting the production of selected potential pollutants. A stepwise linear regression analysis was used to determine the correlation between the operating and production parameters.

A list of the important gasifier operating parameters is shown in Table 20. These were used as the independent variables in correlating the pollutant production parameters which were considered to be the dependent variables in the analysis. The operating parameters were chosen from a more extensive set using engineering judgment and past experience in analyzing gasifier data. Of the 20 variables, 14 characterize the coal used in the tests and the remainder describe the operation of the gasifier. The heating rate during pyrolysis (HTRT), air-to-coal (AC) and steam-to-coal (SC) ratios, and bed temperature (TMAXAVG) are known to affect both the quantity and distribution of products from gasifiers. The amount of coal charged (CLCHRG) and the average gas flow into the gasifier (TGAS) were chosen as independent variables because they are indicative of gas-solid contacting and bed height.

5.1 LINEAR REGRESSION TECHNIQUE[13]

Selected pollutant production variables along with several other indicators of gasifier performance, which make up the dependent variable set, are shown in Table 21. In general, the pollutant production parameters are yields for a specific compound per unit of carbon gasified, or coal loaded. They were chosen because the raw product gas concentration of these compounds typically exceeded published thresholds for adverse health effects.

The stepwise linear regression analysis was carried out using a standard statistical program. Briefly, the stepwise computer program finds the single-variable model which produces the largest R^2 statistic (where R^2 is the square of the multiple correlation coefficient). After entering the variable with the largest R^2, the program uses the partial correlation coefficients to select the next variable to enter the regression. That is, the program enters the variable with the highest partial correlation coefficient (given that the variable with the largest R^2 is already in the model.) An F test is performed

Table 20. IMPORTANT GASIFIER OPERATING PARAMETERS
(Independent Variables in the Regression Analysis)

PCTVOLMT	:	Percent volatile matter in coal.
PCTASH	:	Percent ash in coal.
SULFUR	:	Total percent sulfur in coal.
HTRT	:	Heating rate of the coal during pyrolysis phase taken as the slope of the time temperature curve as the coal is heated from 300°C to 700°C.
AC	:	Air-to-coal ratio (g/g).
AS	:	Air-to-steam ratio (g/g).
PCTMOIST	:	Percent moisture in coal.
FBTULB	:	Higher heating value of coal.
CLCHRG	:	Coal charged to the gasifier (g).
TGAS	:	Average gas flow rate into gasifier (slpm).
TMAXAVG	:	Mean of the maximum bed temperature averaged over the entire test, °C.
ORG	:	Percent organic sulfur in coal.
SULFATE	:	Percent sulfur as sulfate in coal.
SC	:	Steam-to-coal ratio (g/g).
FXDCAR	:	Percent fixed carbon in coal.
PYR	:	Percent sulfur as pyrites in coal.
CARBON	:	Percent carbon in coal.
HYDRO	:	Percent hydrogen in coal.
OXY	:	Percent oxygen in coal.
NITRO	:	Percent nitrogen in coal.

Table 21. IMPORTANT POLLUTION PRODUCTION PARAMETERS AND GASIFIER PERFORMANCE VARIABLES (Dependent Variables In The Regression Analysis)

SCFLB	:	Total gas produced (scf/lb coal)
BTUSCF	:	Higher heating value of gas produced (Btu/scf)
ORACL	:	Tar organic acid yield (g x 100/g coal)
ORBCL	:	Tar organic base yield (g x 100/g coal)
NPNCL	:	Tar nonpolar neutral yield (g x 100/g coal)
PNACL	:	Tar polynuclear aromatic yield (g x 100/g coal)
PCTTARCL	:	Percent tar yield from coal
AR4	:	Tar arsenic yield (µg/g carbon converted)
SU2	:	Ash sulfur yield (µg/g carbon converted)
BEN10	:	Benzene production (µg in bulb/g carbon converted)
BTX	:	BTX production (µg/g carbon converted)
PHET	:	Total phenol production (µg/g carbon converted)
CRET	:	Total cresol production (µg/g carbon converted)
HS10	:	H_2S yield in gas (µg/g carbon converted)
CS10	:	COS yield in gas (µg/g carbon converted)
SRAT10	:	Ratio H_2S to COS in gas (g/g)
MTH10	:	CH_3SH yield in gas (µg/g carbon converted)
NAPT	:	Total naphthalene yield (µg/g carbon converted)
PTHT	:	Total phenanthrene yield (µg/g carbon converted)
INE8	:	Indene yield in gas (g/g carbon converted)
BFU8	:	Benzofuran yield in gas (µg/g carbon converted)
FTH4	:	Fluoranthene yield in tar (µg/g carbon converted)
FLU4	:	Fluorene yield in tar (µg/g carbon converted)

to determine if the variable to be entered has a probability greater than the specified significance level for entry into the analysis. (For the analysis presented here this level was 50 percent.) After a variable is added, the program searches all the variables already included in the model and computes a partial F-statistic to determine if these variables should remain in the model. Any variable not producing a partial F significant at the specified significance level for retention, i.e., 0.10, is then deleted from the model. The process then continues by determining if any other variables should be added to the regression. The process terminates when no variable meets the conditions for inclusion or when the next variable to be added to the model is the one previously deleted from it.

5.2 STATISTICAL ANALYSIS RESULTS: PHASE I

The results of the analysis using the independent variables from Table 20 and the dependent variables in Table 21 are summarized in Table 22. Entrees in this table correspond to the order of importance of each independent variable in accounting for the variation in each dependent variable. For example, in the row labeled "SCFLB" (total scf of product gas per lb coal) a value of 1 was entered in column "AC" (air-to-coal ratio.) This means that the air-to-coal ratio was the most important parameter in correlating the total product gas. Also from the same row it can be seen that the steam-to-coal ratio was the second most important variable in correlating the total product gas with a linear model.

The positive or negative sign following each numerical entree in Table 22 is the sign of the coefficient of the corresponding independent variable in the linear model. For example, examination of the first two dependent variables shows that the volume of product gas increases and the heating value of the gas decreases with increase in air-to-coal ratio. This is to be expected due to increased nitrogen concentration in the product gas.

In order to identify the most important variables affecting pollutant production, the most important independent variables in determining each of the dependent variables (dependent variables with an R^2 less than 0.500 were not considered) shown in Table 22 were assigned the value of V equal to seven minus its ranking in any specific correlation giving an overall ranking index W which gives a measure of the overall importance of that variable in affecting pollutant production.

TABLE 22. SUMMARY OF THE STATISTICAL ANALYSIS OF THE RTI GASIFIER SCREENING RUN USING ALL INDEPENDENT VARIABLES IN TABLE 20

Dependent Variables	Independent Variables																					R^2	No. Observations
	% vol. matter (PCTVOLMT)	% ash (PCTASH)	% sulfur (SULFUR)	heating rate (HTRT)	air/coal (AC)	air/steam (AS)	% moisture (PCTMOIST)	heating value (FBTULB)	coal charged (CLCHRG)	inlet gas flow (TGAS)	bed temperature (TMAXAVG)	% organic S (ORG)	% sulfate S (SULFATE)	steam/coal (SC)	% fixed carbon (FXDCAR)	% pyritic S (PYR)	% carbon (CARBON)	% hydrogen (HYDRO)	% oxygen (OXY)	% nitrogen (NITRO)		
gas produced (SCFLB)				4-	1+				3+					2+								0.965	34
gas HHV (BTUSFC)				3+	1-									2+								0.766	25
organic acids (ORACL)	1+									2+	3-											0.662	19
organic bases (ORBCL)	2+		1+		7+				3+		6-			5+							4+	0.981	19
nonpolar neutrals (NPNCL)	2+															1+						0.338	19
PNAs (PNACL)		5+	2+	1+					4+	3-												0.876	18
tar yield (PCTTARCL)	2+								3+							1+						0.850	19
arsenic in tar (AR4)			1+						2+													0.768	8
sulfur in ash (SU2)					2+								1+					3+				0.688	18
benzene yield (BEN10)			1+	4+		3-		2+														0.838	17
BTX yield (BTX)				3+						2-	4+			1+							5-	0.958	15
phenol yield (PHET)																					1-	0.346	14
cresols yield (CRET)									1-													0.456	14
hydrogen sulfide (HS10)											2-					1+						0.715	21

(continued)

Table 22 (continued).

Dependent Variables	Independent Variables: % vol. matter (PCTVOLMT)	% ash (PCTASH)	% sulfur (SULFUR)	heating rate (HTRT)	air/coal (AC)	air/steam (AS)	% moisture (PCTMOIST)	heating value (FBTULB)	coal charged (CLCHRG)	inlet gas flow (TGAS)	bed temperature (TMAXAVG)	% organic S (ORG)	% sulfate S (SULFATE)	steam/coal (SC)	% fixed carbon (FXDCAR)	% pyritic S (PYR)	% carbon (CARBON)	% hydrogen (HYDRO)	% oxygen (OXY)	% nitrogen (NITRO)	R^2	No. Observations
carbonyl sulfide (CS10)					1+								3-	2+	4-						0.862	21
H_2S/COS (SRAT10)						2-				3-			1+								0.731	21
methanethiol (MTH10)													2-	1+							0.334	19
naphthalene (NAPT)												1+									0.416	15
phenanthrene (PTHT)			1+						2+					3-							0.990	7
indene (INE8)											1+										0.098	16
benzofuran (BFU8)						1-					2-										0.513	14
fluoranthene (FTH4)	4+								2+	3-		1+									0.871	16
fluorene (FLU4)												1+									0.261	16

The independent variable(s) of greatest importance were different depending upon the specific dependent variable of interest. Table 22 shows that the sulfur level was of primary importance in the yield of organic tar bases and benzene, both of which are known to have a high level of potential for carcinogenic and/or mutagenic activity. Gasifier operating parameters CLCHRG (coal charged) and TGAS (inlet gas flow rate) were found to be of importance in the production of several pollutants. As discussed previously, these parameters represent the reactor bed height and the conditions of gas-solid contacting. The mechanism(s) through which the parameters identified in Table 23 influence pollutant production is not explicitly known at present. It is possible that mechanisms of pollutant production may not directly involve the identified parameters but that these parameters may be indicative of intermediate processes or parameters not considered in the analysis but which are highly correlated with the identified parameters. A more basic phenomenological study of gasification process would help reveal the relationship between the identified independent parameters and pollutant production rates; such work is planned as a part of this project.

5.3 STATISTICAL ANALYSIS RESULTS: PHASE II

Statistical analyses were performed to determine if the independent parameters shown in Table 23 are significantly correlated with each other. In the case where two variables have a high degree of correlation one can be eliminated from the analysis. A reduction in variables is beneficial in that the linear models for predicting pollutant product yields would involve fewer independent variables. A strategy was developed for reducing redundant variables:

1. Starting with the most important variable as listed in Table 23, variables of lesser importance were eliminated from consideration as a primary parameter if they had a high degree of correlation with the most important variable.
2. Step 1 was repeated throughout Table 23 until no variables were remaining for consideration.

Applying this procedure to Table 23 resulted in the set of primary independent variables listed in Table 24. The stepwise linear regression procedure described above was applied in correlating the pollutant production yields and gasifier performance variables listed in Table 21 with the primary dependent variables in Table 24. The results of this analysis are summarized in Table

TABLE 23. RANKING OF OPERATING PARAMETERS IN THE ORDER OF IMPORTANCE IN INFLUENCING POLLUTANT PRODUCTION

Independent Variable	Ranking Index* W	Overall Importance in Pollutant Formation
% sulfur (SULFUR)	29	1
coal charged (CLCHRG)	25	2
inlet gas flow (TGAS)	22	3
% vol. matter (PCTVOLMT)	19	4
bed temperature (TMAXAVG)	18	5
steam/coal (SC)	17	6
% sulfate S (SULFATE)	16	7
air/steam (AS)	15	8
heating rate (HTRT)	13	9
% pyritic S (PYR)	12	10
air/coal (AC)	11	11
% organic S (ORG)	6	12
heating value (FBTULB	5	13
% nitrogen (NITRO)	5	14
% hydrogen (HYDRO)	4	15
% fixed coal (FXDCAR)	3	16
% ash (PCTASH)	2	17
% moisture (PCTMOIST)	0	18
% carbon (CARBON)	0	19
% oxygen (OXY)	0	20

*The overall ranking index, W, is the sum of the V values from the individual correlations, where V is seven minus the ranking of the independent variable under consideration.

TABLE 24. RANKING OF THE MOST IMPORTANT, INDEPENDENT OPERATING PARAMETERS INFLUENCING POLLUTANT PRODUCTION

Independent Variable	Ranking Index* W	Overall Importance in Pollutant Production
% sulfur (SULFUR)	40	1
% sulfate S (SULFATE)	24	2
% vol. matter (PCTVOLMT)	22	3
steam/coal (SC)	21	4
coal charged (CLCHRG)	20	5
inlet gas flow (TGAS)	18	6
bed temperature (TMAXAVG)	16	7
air/steam (AS)	15	8
air/coal (AC)	12	9
heating rate (HTRT)	8	10

*The overall ranking index, W, is the sum of the V values from the individual correlations, where V is seven minus the ranking of the independent variable under consideration.

25. (The entries in this table have the same significance as described for Table 22.) An overall ranking of importance of the dependent variables in affecting pollutant production was again performed. The results of this ranking are shown in Table 24.

The linear models for pollutant yields and gasifier performance using the dependent variable listed in Table 24 are shown in Table 26. The entries in the columns of this table are coefficients of the corresponding independent variables in the linear model of the dependent variable. For example, the product gas yield is given by

SCFLB = -12.23 + 3.928*SC + 0.01611*CLCHRG + 19.12*AC-0.1472*HTRT.

Relative to the yields of potential pollutants considered in this analysis, the coal characterization parameters of total sulfur, sulfate and volatile content were the most important parameters. The importance of the volatile matter content of the raw coals undoubtedly reflects the fact that the coal-derived volatiles contain many of the potential pollutants under study here. The three sulfur variables of total sulfur, pyritic sulfur, and organic sulfur were found to exhibit generally the same behavior in the regression analyses. This is explained by the fact that the pyritic sulfur and organic sulfur levels were highly correlated with the total sulfur level, the correlation coefficients being 0.90 and 0.85 respectively.

The importance of sulfur indicated in Tables 24 and 26 may to some extent be the result of statistical bias which lacks physical meaning. However, an attempt to further evaluate the possible existence of causative factors has been initiated. The sulfur species, viz., pyritic, organic, and/or total sulfur content, were intercorrelated as independent variables relative to dependent variables as hydrogen sulfide yield, etc. Moreover, the iron content of the coal is highly correlated with the pyritic sulfur. Iron is capable of substituting for sulfur in thiophene structures; thus, a higher iron pyrite content for coal can result in a greater potential for the modification of organically bonded sulfur.

Also, sulfur is known to form thia- and dithiaether linkages in hydrocarbon media. This can be a form of "vulcanization" in which the presence of the sulfur promotes the formation and/or maintenance of larger molecular

TABLE 25. SUMMARY OF THE STATISTICAL ANALYSES OF THE RTI GASIFIER USING THE MOST IMPORTANT, INDEPENDENT OPERATING VARIABLES

Dependent Variables	Independent Variables										R^2	No. Observations
	% vol. matter (PCTVOLMT)	% sulfur (SULFUR)	heating rate (HTRT)	air/coal (AC)	air/steam (AS)	coal charged (CLCHRG)	inlet gas flow (TGAS)	bed temperature (TMAXAVG)	% sulfate S (SULFATE)	steam/coal (SC)		
gas produced (SCFLB)			4-	1+		3+				2+	0.965	34
gas HHV (BTUSFC)			3+	1-						2+	0.766	25
organic acids (ORACL)	1+						2+	3-			0.662	19
organic bases (ORBCL)	1+	2+		6-	3-	4+		5-			0.955	19
nonpolar neutrals (NPNCL)	1+				2-						0.313	19
PNAs (PNACL)		1+	2+			4+	3-				0.777	17
tar yield (PCTTARCL)	1+	2+				3+			4+		0.860	19
arsenic in tar (AR4)		1+				2+					0.768	8
sulfur in ash (SU2)				2+					1+		0.608	18
benzene yield (BEN10)	3+		4+				2-			1+	0.878	17
BTX yield (BTX)									2-	1+	0.710	15
phenol yield (PHET)										1+	0.251	14
cresols yield (CRET)						1-					0.456	14
hydrogen sulfide (HS10)		1+						2-			0.701	21
carbonyl sulfide (CS10)				1+					3-	2+	0.801	21
H_2S/COS (SRAT10)					2-		3-		1+		0.731	21
methanethiol (MTH10)									2-	1+	0.334	19

TABLE 25 (continued).

Dependent Variables	Independent Variables											R^2	No. Observations
	% vol. matter (PCTVOLMT)	% sulfur (SULFUR)	heating rate (HTRT)	air/coal (AC)	air/steam (AS)	coal charged (CLCHRG)	inlet gas flow (TGAS)	bed temperature (TMAXAVG)	% sulfate S (SULFATE)	steam/coal (SC)		
naphthalene (NAPT)		1+										0.323	15
phenanthrene (PTHT)		1+				2+				3-		0.990	7
indene (INE8)								1+				0.091	16
benzofuran (BFU8)					1-			2-				0.513	14
fluoranthene (FTH4)		1+										0.555	16
fluorene (FLU4)								1+				0.261	16

TABLE 26. SUMMARY OF LINEAR MODELS FOR POLLUTION PRODUCTION AND GASIFIER PERFORMANCE

	ORACL	ORBCL	PNACL	PCTTARCL
INTERCEPT	9.623E-1	3.155E-2	- 9.817E-1	- 5.916
INDEPENDENT VARIABLES				
SULFUR	--	3.372E-2	3.474E-1	4.694E-1
SULFATE	--	--	--	5.447
PCTVOLMT	1.815E-2	4.950E-3	--	1.014E-1
SC	--	--	--	--
CLCHRG	--	1.123E-4	7.792E-4	2.315E-3
TGAS	7.733E-3	--	- 1.516E-2	--
TMAXAVG	- 1.456E-3	- 2.682E-4	--	--
AS	--	- 2.319E-2	--	--
AC	--	1.510E-2	9.913E-3	--
HTRT	--	--	--	--
R^2	0.662	0.955	0.777	0.860
No. Observations	19	19	18	19

	AR4	SU2	BEN10	BTX
INTERCEPT	- 1.159E-3	- 1.791E+1	-5.372E+3	8.350E+3
INDEPENDENT VARIABLES				
SULFUR	2.378E-4	--	--	--
SULFATE	--	1.399E+2	2.585E+2	- 2.420E+4
PCTVOLMT	--	--	--	--
SC	--	--	7.195E+3	1.084E+4
CLCHRG	7.500E-7	--	--	--
TGAS	--	--	- 2.172E+2	--
TMAXAVG	--	--	--	--
AS	--	--	--	--
AC	--	5.632	1.184E+2	--
HTRT	--	--	--	--
R^2	0.768	0.608	0.878	0.710
No. Observations	8	18	17	15

continued

TABLE 26 (continued).

	HS10	CS10	PTHT	BFU8
INTERCEPT	1.148E+5	- 8.406E+2	- 1.462E+1	1.459E+3
INDEPENDENT VARIABLES				
SULFUR	1.502E+4	--	1.388	--
SULFATE	--	- 4.962E+3	--	--
PCTVOLMT	--	--	--	--
SC	--	3.639E+2	- 4.332E-1	--
CLCHRG	--	--	9.725E-3	--
TGAS	--	--	--	--
TMAXAVG	- 1.242E+2	--	--	- 1.120
AS	--	--	--	- 7.813E+1
AC	--	9.352E+2	--	--
HTRT	--	--	--	--
R^2	0.701	0.801	0.990	0.513
No. Observations	21	21	7	14

		FTH4	SCFLB	BTUSCF
INTERCEPT		- 1.482E-5	- 1.223E+1	1.990E+2
INDEPENDENT VARIABLES				
SULFUR		1.490E-4	--	--
SULFATE		--	--	--
PCTVOLMT		--	--	--
SC		--	3.928	2.143E+1
CLCHRG		1.611E-2	--	--
TGAS		--	--	--
TMAXAVG		--	--	--
AS		--	--	--
AC		--	1.912E+1	- 5.963E+1
HTRT			- 1.472E-1	9.628E-1
R^2		0.555	0.965	0.766
No. Observations		16	34	25

weight hydrocarbons, i.e., tars. Clearly, the sulfur, nitrogen, and oxygen content of gasifier tar precursors influences its chemical properties.

The most important gasifier operating variable affecting pollutant production was the steam-to-coal ratio. This variable had a significant influence on benzene and total BTX production. (The steam may have functioned to reduce the oxygen partial pressure in the reactor during the devolatilization, i.e., unsteady-state, period. This phenomenon should not occur in a continuous fixed-bed gasifier). The other operating variables except the heating rate listed in Table 24 also had about the same order of significance in influencing pollutant production as did the steam-to-coal ratio. Heating rate was only found to be influential in the yield of tar PNA.

The height of the coal bed in the RTI laboratory gasifier was also found to have some statistical influence on various of the output (dependent) variables, as measured by the coal charge quantity (CLCHRG). This is probably a result of the fact that a greater bed height reduces the zone above the bed where residence time and thermal conditions are favorable to the cracking or gasification of tars and oils, for example. Hence, as the coal charge quantity increases the yield of tar, for example, may increase, as was found in this study.

In Figures 12 through 16, the predicted yields for several pollutants are compared to the experimental values obtained from the RTI gasifier. It can be seen that the agreement is reasonable even though the gasifier runs include a variety of coals and operation conditions.

The predicted yield of organic bases (ORBCL) in crude gasifier tar is shown in Figure 12 versus the actual yield. A correlation coefficient of 0.955 was obtained. Six independent variables appear in the correlation, as shown in the second column of Table 26. The amount of scatter in the data is seen to be quite low and uniform over the range of the correlation for the 19 values available.

The predicted polynuclear aromatics (PNACL) yield in crude gasifier tar is shown in Figure 13 versus the actual yield. The noticeable degree of scatter seen in this figure is reflected by a correlation coefficient of 0.777. As seen in Table 26, the three independent variables which most successfully represent the yield of polynuclear aromatics are coal sulfur content (SULFUR), coal charge amount (CLCHRG), the gas flow rate (TGAS) to

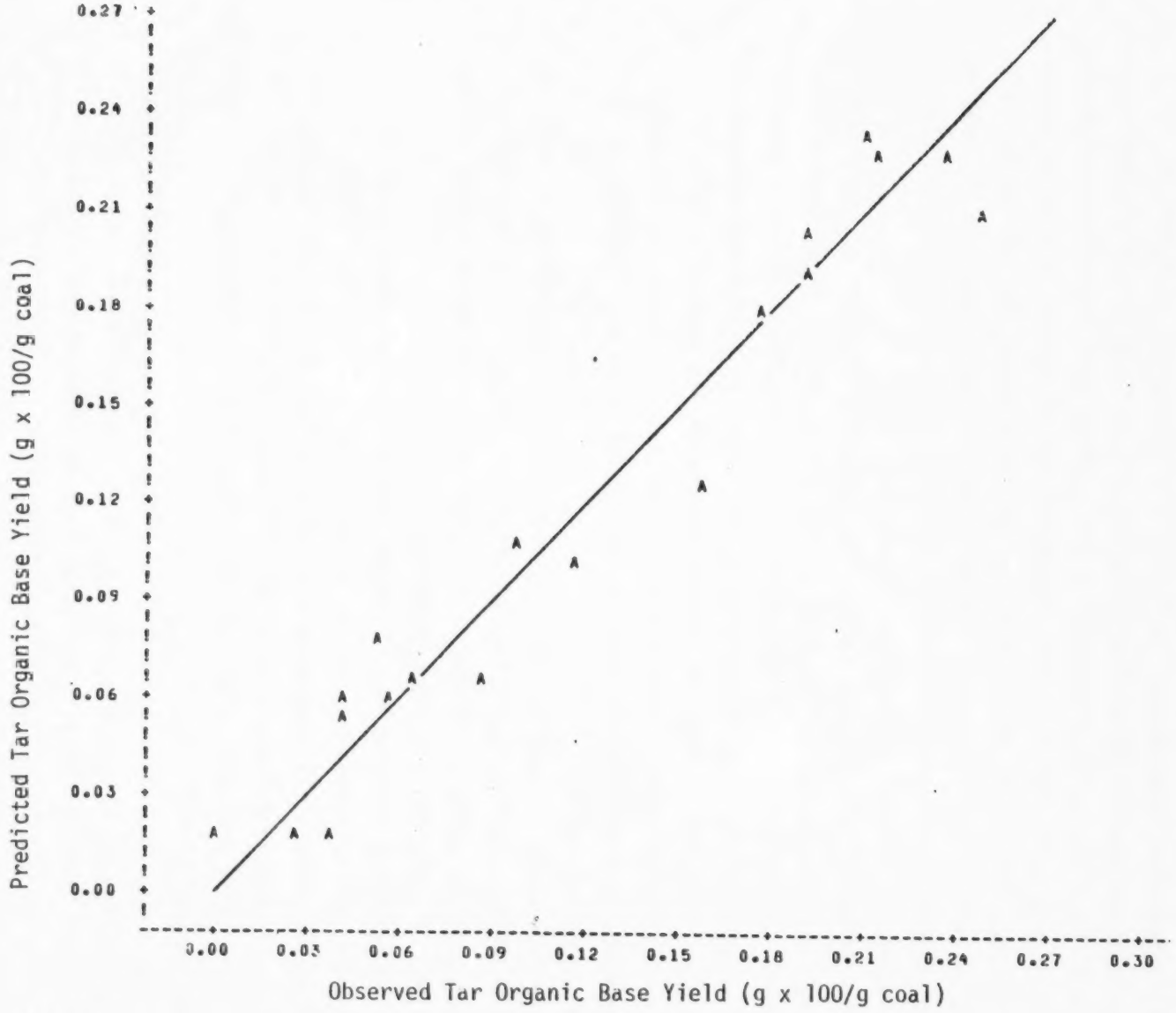

Figure 12. Comparison of the observed and predicted tar organic base yields for the RTI gasifier screening tests.

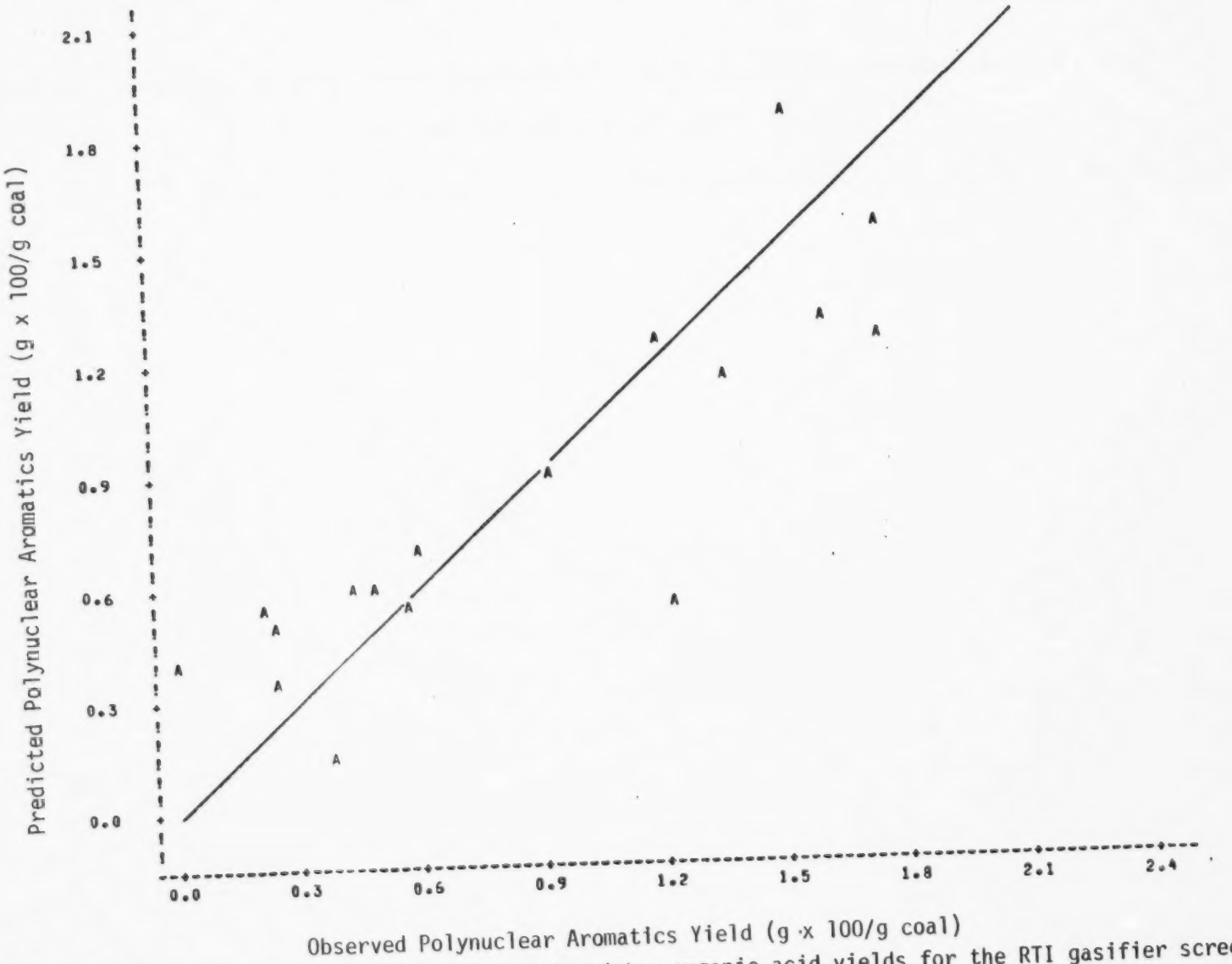

Figure 13. Comparison of the observed and predicted tar organic acid yields for the RTI gasifier screening tests.

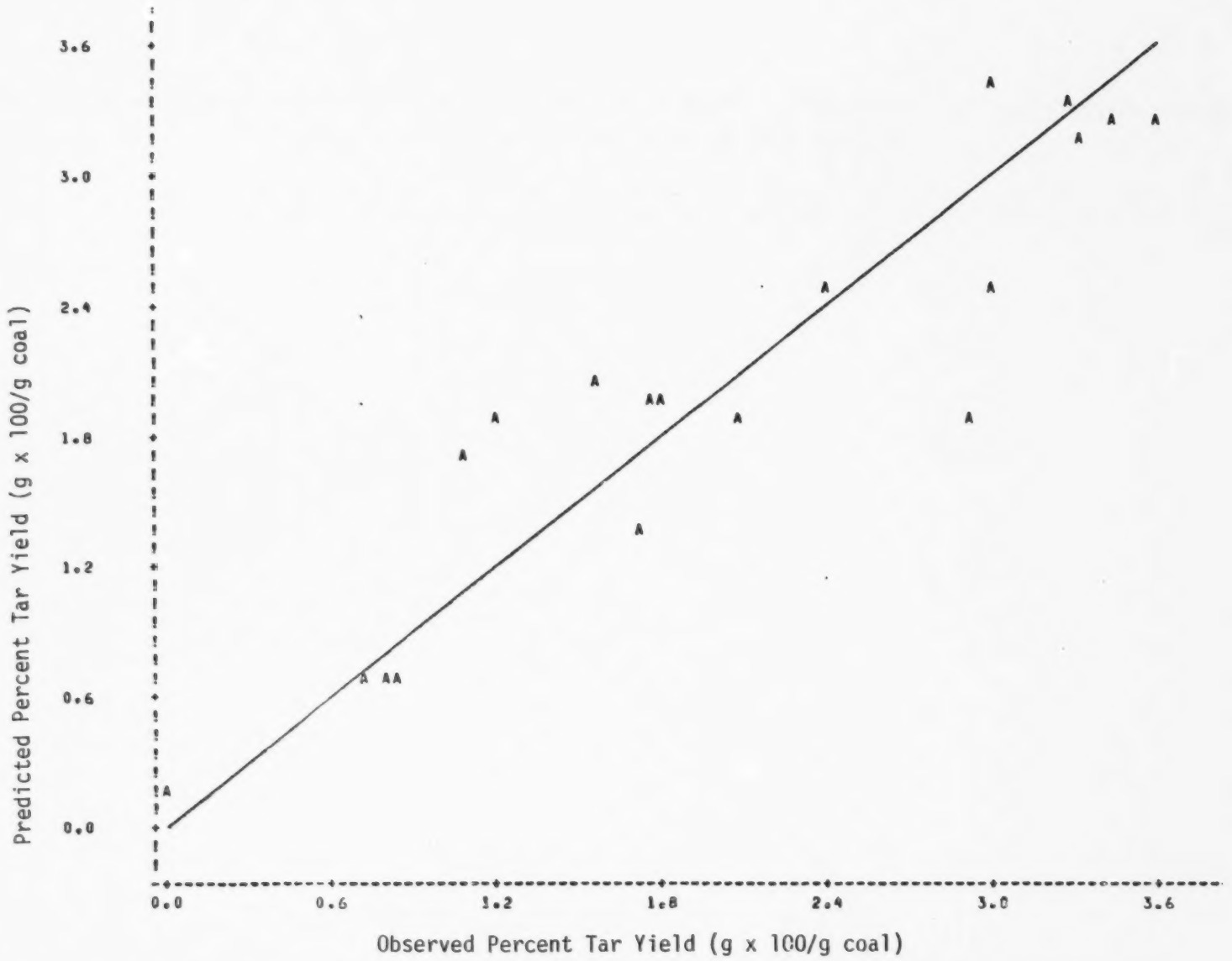

Figure 14. Comparison of observed and predicted tar yields for the RTI gasifier screening tests.

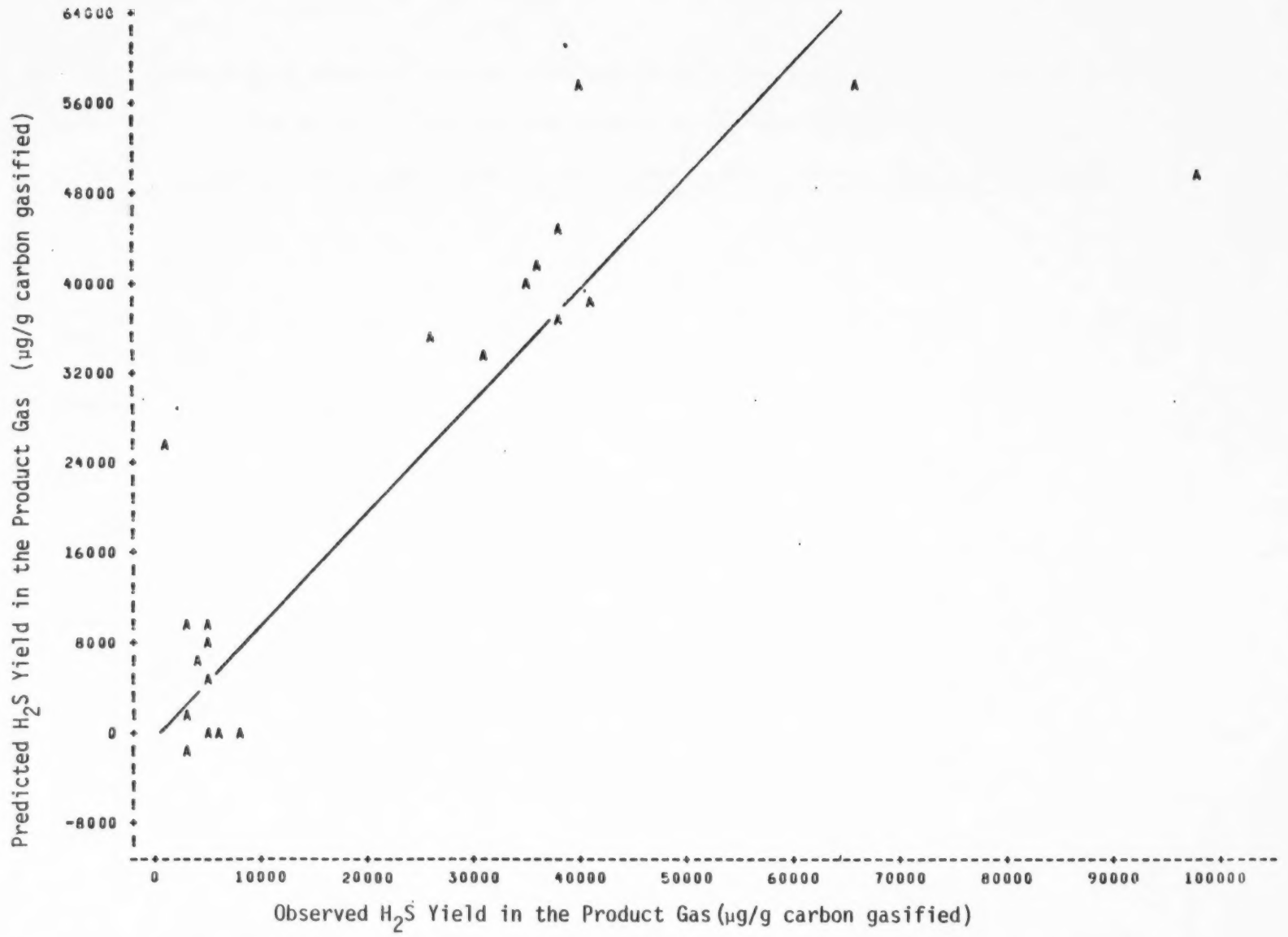

Figure 15. Comparison of observed and predicted H_2S yields for the RTI gasifier screening tests.

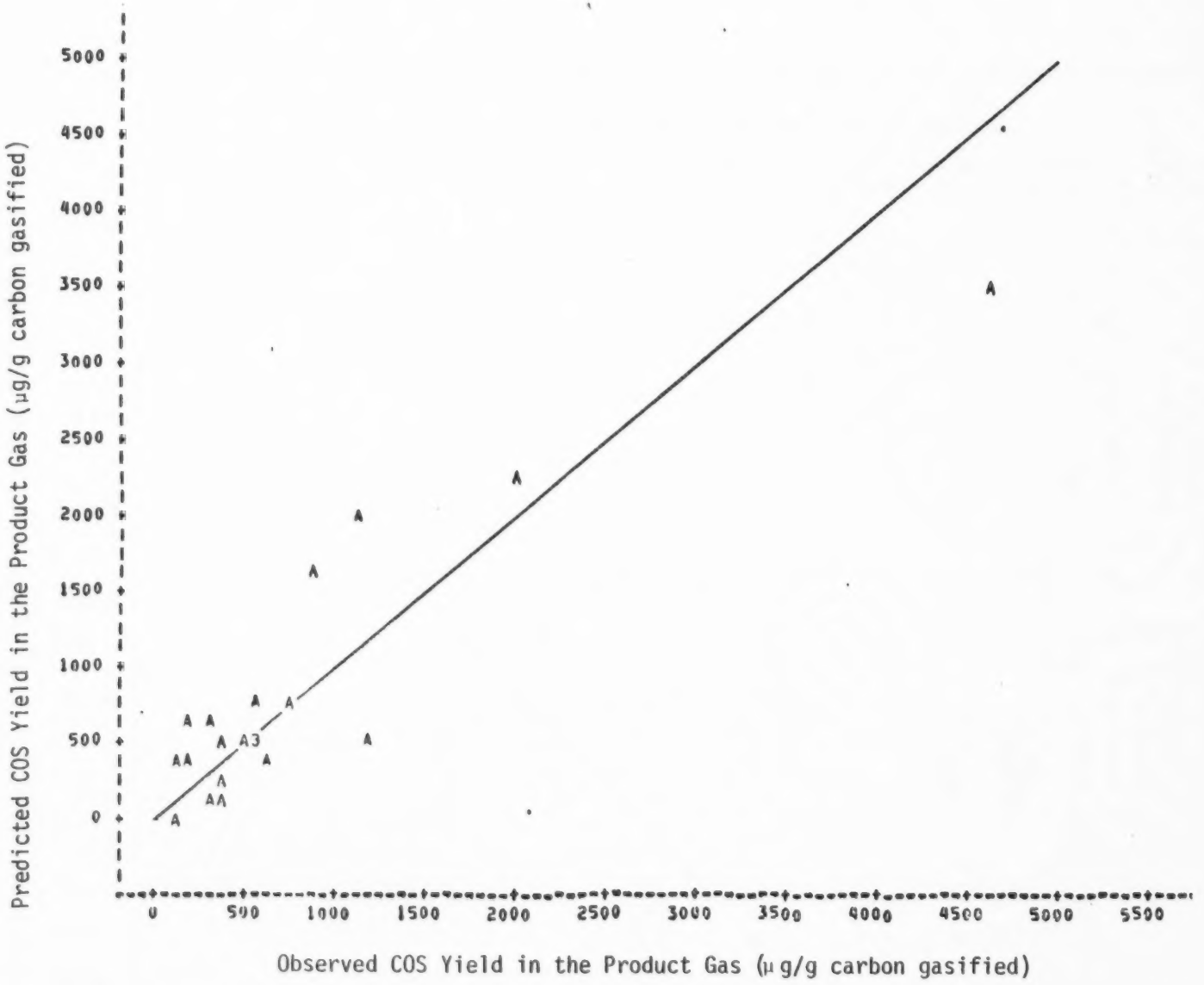

Figure 16. Comparison of observed and predicted COS yields for the RTI gasifier screening tests.

the gasifier, and the air/coal feed ratio (A/C). (One of the observations is not shown on Figure 13 as it was off-the-scale used.)

Figure 14 displays the predicted versus observed yield of crude gasifier tar (PCTTARCL), expressed as percent of the raw coal feed which appears as tar, i.e., grams tar x 100/grams coal. A good correlation was obtained; the correlation coefficient was 0.860 based on four significant independent variables. These were the total sulfur (SULFUR), sulfate sulfur (SULFATE), percent volatile matter (PCTVOLMT), and quantity of coal used (CLCHRG).

The yield of hydrogen sulfide is displayed in Figure 15 where the predicted values are plotted versus the measured values. Some 20 of the 21 observations are shown, one being off-scale. The degree of scatter is reasonably low (correlation coefficient = 0.701); one point is seen to be at an extreme value and could be considered an "outlier." The hydrogen sulfide yield was found to be higher when the total sulfur level of the raw coal was higher and lower when the reactor bed temperature was lower.

The carbonyl sulfide yields were always secondary to those for hydrogen sulfide by about two orders of magnitude. A reasonably good correlation coefficient (R^2 = 0.801) resulted for the carbonyl sulfide yield in terms of the sulfate, steam/coal ratio and air/coal ratio, as shown in Table 26. However, it is seen in Figure 16 that the data are heavily grouped near the low end of the range of yield values. Probably the most significant aspects are that (a) the carbonyl sulfide yield did not vary substantially, even with wide variations in the total sulfur content of the feed coal, and (b) the yield level was well-correlated by three variables each of which provide measures of oxygen input to the gasifier. (This latter condition may indicate that carbonyl sulfide is formed primarily via secondary reactions, for example from hydrogen sulfide interactions with oxygen and oxides of carbon. It is generally known that the reaction of H_2S and CO to form COS and H_2 tends to be near an equilibrium condition in the raw product gas from a coal gasifier. This latter condition is consistent with the general concentration levels observed, i.e., the H_2S/COS ratio was in the range of 20 to 200 typically.)

6.0 CONCLUSIONS

The objective of this project is to develop a fundamental understanding of those factors which influence the production of potential environmental pollutants in synfuel processes. This information is needed to provide guidance for the control of potentially harmful pollutants from future synfuels plants.

A series of screening tests have been completed using a laboratory scale gasification reactor. The purpose of these screening tests was to compare pollutants, qualitatively and quantitatively, from a variety of coals under similar gasification conditions. Coals tested were Montana Rosebud, Wyoming subbituminous, North Dakota Lignite, Pittsburgh No.8, Illinois No.6, Western Kentucky No.9, and FMC char. Chemical analyses of the coals, particulate residues, tars, aqueous condensates, primary gaseous products, and volatile organics have been performed. Emphasis has been upon determination of the organic constituents in the effluent streams.

The laboratory reactor has been operated primarily as a nonisothermal pollutant generation facility. Steam furnaces have been utilized to provide a primary reactant to the bottom of the vertical reaction chamber. Also, pressurized air and/or oxygen have been supplied for reaction. The air-to-steam ratios have been controlled so as to achieve operating conditions representative of practical gasifier operation. Further, both the steam and air rates have been controlled so that the coal bed temperature is maintained at desirable levels. In this way, successful operation of the reactor has been achieved while operating with simultaneous temperature control; this is provided through use of a three-zone electric furnace which surrounds the reactor. Data collection has been possible as a result of the utilization of a PDP 11/34 signal processing system operated on-line with the reactor facility.

High carbon conversions have been achieved as desired. Higher rank coals showed slightly less carbon conversion; they possess a somewhat lower reactivity. Also, the conversion of the sulfur species in the feed coal have been generally above 80 percent during gasification runs to approximately 1000°C. It has been concluded that the level of sulfur conversion can be increased if the overall residence time for reaction exceeds that required for carbon conversion alone. However, the screening test runs were terminated once oxygen was detected in the gas exit stream.

Two distinct time phases for reaction were observed in the screening test runs. These have been characterized as surge and steady-state periods. The surge period involves devolatilization of the coal and represents the conditions under which effluent concentrations vary substantially with time. After the methane concentration in the effluent gas has dropped below approximately two volume percent, it has been observed that the temperature and concentration of the effluent stream is generally well behaved, i.e., steady-state. It is believed that this phase involves primarily the gasification of char via the carbon/steam reaction, the partial oxidation of carbonaceous material, and the carbon/carbon dioxide reaction. The supporting evidence for the understanding of reactor behavior and characterization of pollutant production has been obtained as a result of using sampling and analysis techniques which have been specifically developed for these studies.[2]

Application of these testing methods have provided concentrations and amounts for the reactor residue, aqueous condensate, oils and tar, as well as the primary gas product stream. This stream has been subjected to routine gas chromatographic analysis as well as infra-red measurements so as to successfully maintain known and desirable operating conditions within the facility. Relative quantities of organic pollutants have resulted from these tests. For convenience, these results have been expressed as mass of compound produced from each effluent per unit of feed carbon converted within the reactor. The dominant compounds which have been identified in the effluent streams are hydrogen sulfide, carbonyl sulfide, phenol, cresols, benzene, toluene, naphthalene, anthracene, and phenanthrene. Additional studies are currently underway to characterize the tar fractions relative to the wide distribution of compounds which are contained therein.

The Western Kentucky No.9 and Illinois No.6 coals were found to generate larger tar yields, while subbituminous and lignite coals resulted in somewhat less tar production. The smallest yield of PNA and organic base materials were obtained from North Dakota lignite, while the largest yields resulted from Western Kentucky No.9 coal. Generally, the tar yields were found to be substantial during these runs. This is in agreement with the tar yields of commercial fixed bed coal gasifiers operating with medium and high volatile coal feed materials.[14,15]

Trace element studies have indicated that arsenic, cadmium, lead and mercury may also generally be volatilized during gasification. (Additional results on trace element analyses have recently been obtained via neutron activation analysis techniques. While the results are generally in agreement with those of atomic absorption, both sets have revealed that measurements of the trace elements being carried by the primary gas stream may be necessary to fully account for the fate of these elements within the gasification process.

Material balance calculations have been completed for many of the screening test runs. It was generally difficult to achieve a high degree of closure on material balances for the semibatch tests as they were conducted over extended time periods. However, overall closure was obtained for these runs at a level well within a standard deviation of only 13 percent. Closure was obtained least well for sulfur, ash, and hydrogen. (It has been demonstrated that the percentage closure for the individual elements can be substantially improved by adjusting the material balances so as to force closure on a selected element, e.g., oxygen. This condition indicates that some experimental error is present in the results which is due, perhaps, to inaccuracies in the overall determination of gas flow rates.)

A statistical analysis of the RTI gasifier screening runs was carried out to identify the most important operating parameters affecting the production of selected pollutants. Specifically, a stepwise linear regression analysis was used to determine the correlation between the operating and production parameters. Some 20 operating variables were chosen for analysis. In the production of potential pollutants, the coal characterization parameters of total sulfur, sulfate and volatile content were the most important quantities in determining yields. Total sulfur was indicated to significantly affect the production of both sulfur and nonsulfur compounds. The most important gasifier operating variable affecting pollutant production was the steam-to-coal ratio. This variable had a significant influence on benzene and total BTX production. A number of other operating variables were also of significance in influencing pollutant production. Heating rate was found to be influential in the yield of the PNA fraction of the tar.

The statistical analysis also showed that increases in both the air-to-steam ratio and the bed temperature decreased the yield of several of the major pollutants. However, no significant correlation existed between the

selected independent variables and the yields of phenol and naphthalene. Since phenol is the primary pollutant in the gasifier condensate, a mechanistic approach to explaining the production of phenol rather than the statistical approach is warranted.

The screening test runs have been extremely useful in providing operating experience with a unique experimental facility. The simultaneous function of the reactor facility, signal processing system, and sampling system has required check-out procedures and numerous troubleshooting tasks. The successful operation of a gasification process in which feed materials and operating variables are intentionally being changed for experimental purposes gives rise to complexities in chemical process control. However, a versatile system has been established and prepared for parametric test runs.

Parameters for gasification tests are pressure, temperature, coal particle size, reactant flow rates, and coal additives. Hence, operation of the test facility under carefully controlled conditions in which specifically determined variables are set at preselected values will be performed and analyzed. This is intended to provide basic data for the understanding of pollutant formation during coal gasification.

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APPENDICES

I. Signal Processing System

II. Pollutant Production Factors

APPENDIX I

SIGNAL PROCESSING SYSTEM

The laboratory reactor facility which has been used to study coal gasification and pollutant generation is equipped with versatile signal processing and data handling capabilities. The hardware includes an on-line digital processor, i.e., the central processing unit, as well as quick-response accessories. Detectors for temperatures, pressures, flow rates, and chemical compositions are connected directly to the experimental facility, as shown in Figure 17. Signals from these detectors or monitors move directly to the industrial control (remote), i.e., ICR, where signal conversion and conditioning occurs. The ICR is connected directly to the CPU, which is a PDP 11/34. Operator access to the CPU may be achieved via a console at the CPU or a terminal near the experimental system.

Generally, four modes of system operation are in use. The first mode represents "system generation" activities, i.e., software introduction and/or modification. The second operational mode is that of real-time signal processing, i.e., the activity which involves experimental runs on the laboratory gasifier and/or real-time chemical analysis operations using gas chromatographs. Next, the post-experimental data processing activity is conducted. The fourth mode of system function is that of batch processing, i.e., the execution of user prepared programs in source (FORTRAN) language.

The functional states of the signal processing system which are active for the performance of experimental gasification tests are shown in Figure 18. Before the tests, scan condition and display inputs are provided along with test parameters, and load and start instructions. During the gasification tests, data are stored, print and store alarms are activated; and, other user overrides are instituted. Subsequent to each gasification test, a run log is produced and data accumulated during the run are processed to determine average temperatures, flow rates, compositions and other relevant data values. Carbon conversion and steam conversion values are also computed.

Signal processor function in support of gas chromatograph (GC) analyses is also an important component of system use. As shown in Figure 19, various system operations take place before, during, and after the GC analyses. Before GC runs, the operator introduces input parameters and calibration

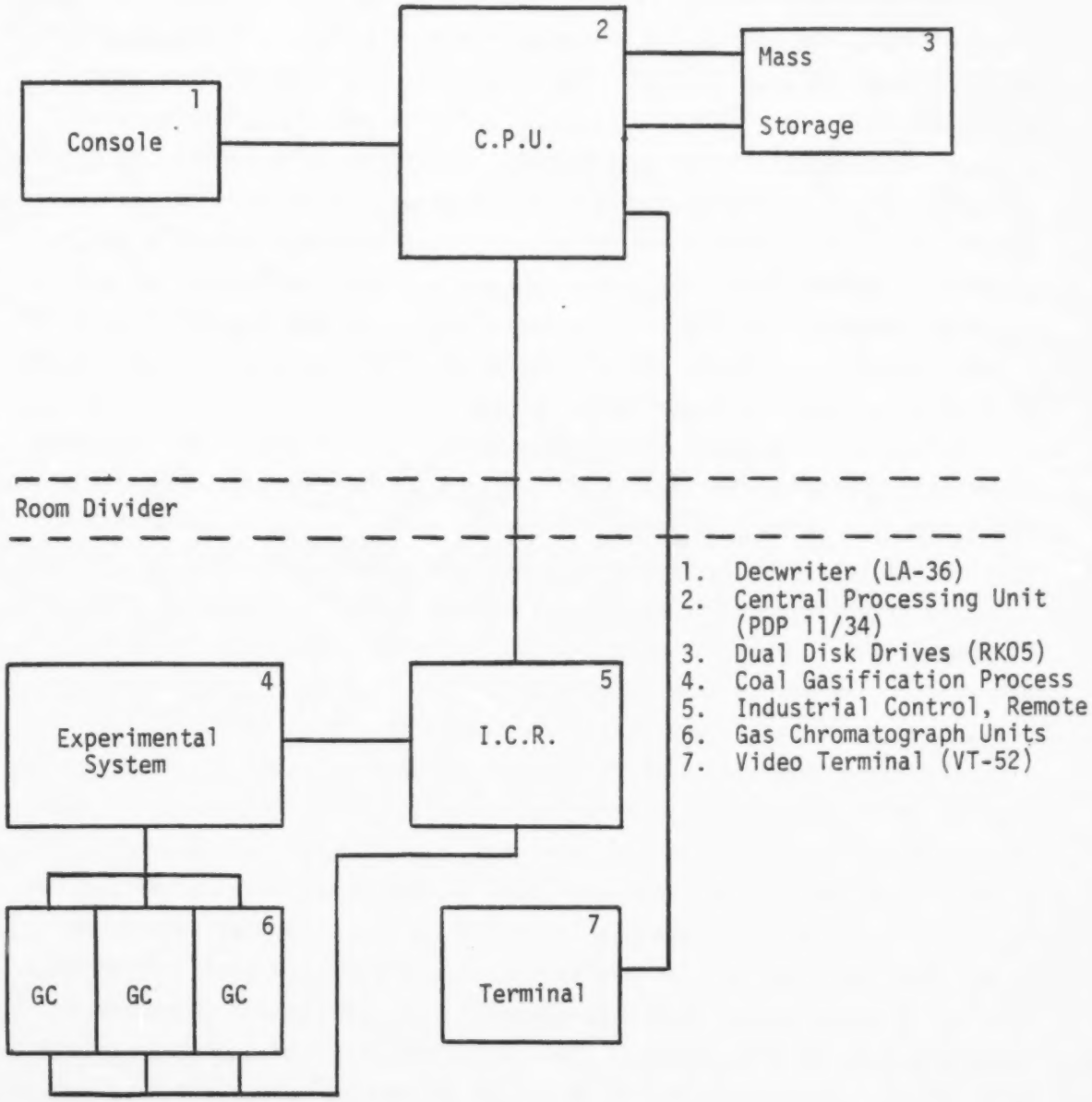

Figure 17. Signal processing hardware configuration.

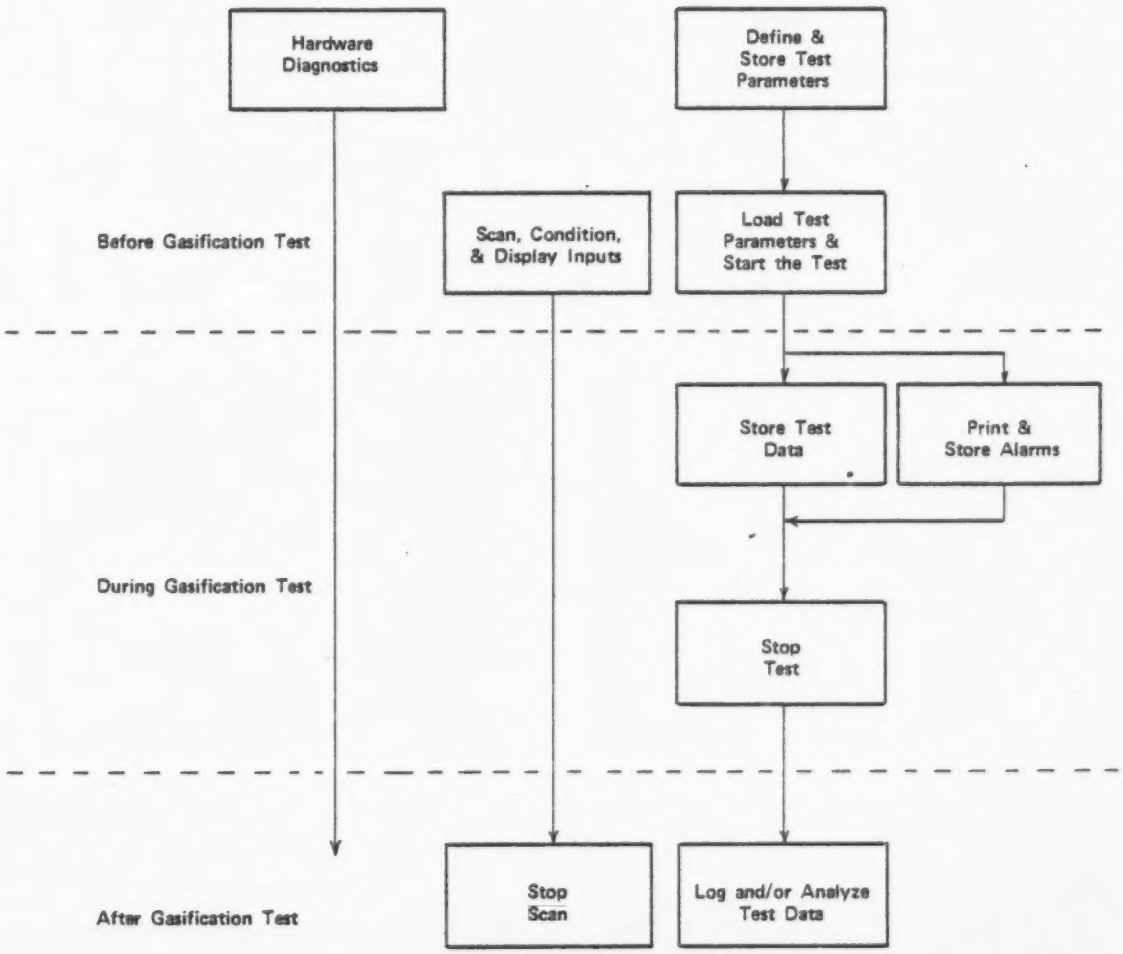

Figure 18. Signal processor function relative to gasification tests.

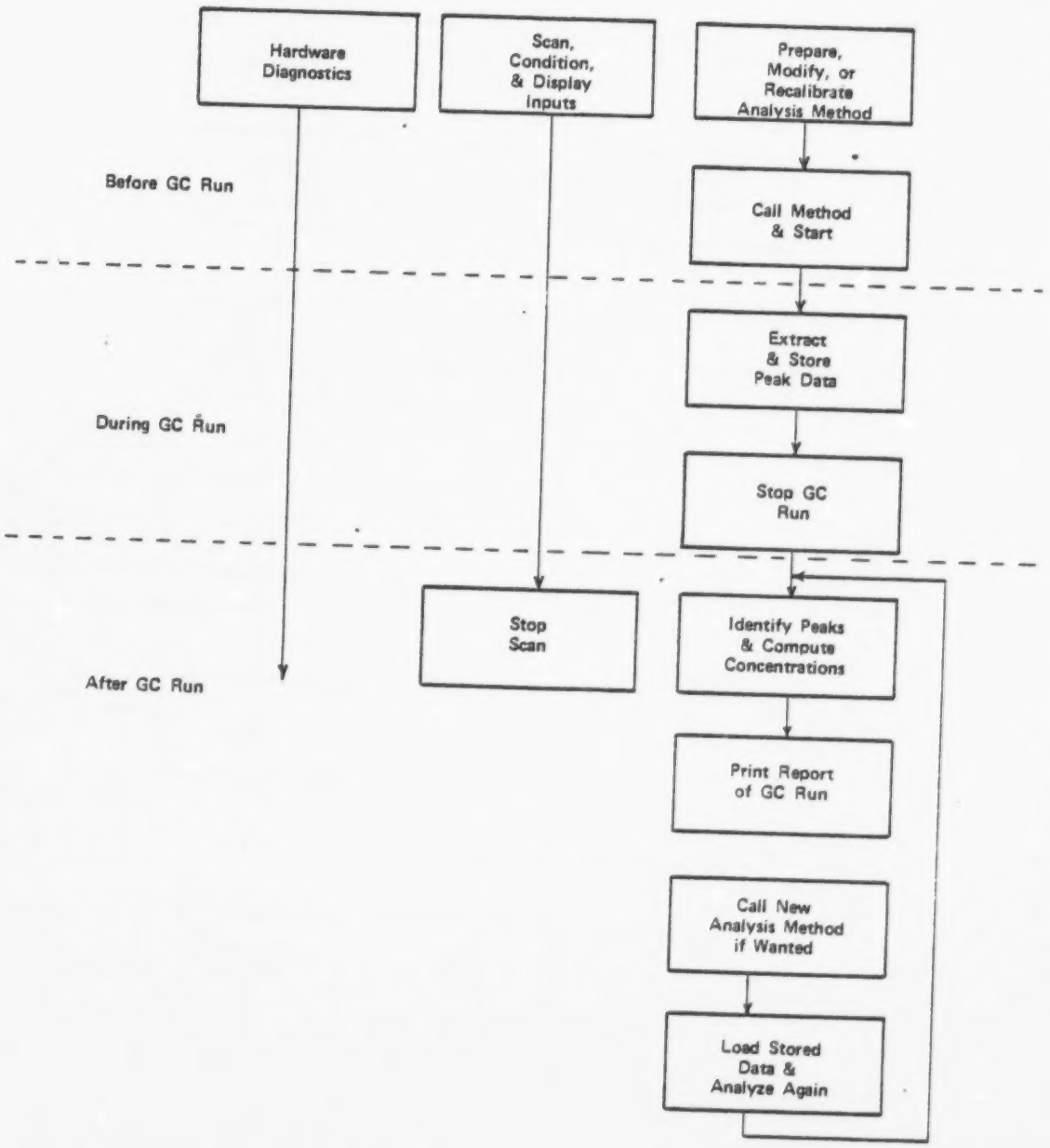
Hardware Diagnostics
Scan, Condition, & Display Inputs
Prepare, Modify, or Recalibrate Analysis Method
Before GC Run
Call Method & Start
Extract & Store Peak Data
During GC Run
Stop GC Run
Stop Scan
Identify Peaks & Compute Concentrations
After GC Run
Print Report of GC Run
Call New Analysis Method if Wanted
Load Stored Data & Analyze Again

Figure 19. Signal processor function relative to GC analyses.

instructions. During operation of the gas chromatographs, the signal processor is receiving input data through an analog/digital converter interface. After the GC run, the signal processing system is activated to determine residence times for compound identification as well as the integration and correction of peak areas for an accurate determination of the concentration of each species being analyzed. Next, a report is printed of the results of the GC runs.

The various software packages which have been prepared in this project in support of gasification test run monitoring, gas chromatograph operation and data analysis are shown in Figure 20. This figure displays the functional interrelations among the software packages and the signal processing system hardware. It may be noted that most of the software serves a supervisory function. As such, these software packages provide the capability for on-line data collection, system monitoring, and process variable manipulation. Thus, accurate and comprehensive data collection can be achieved. Further the continuous monitoring of specific process variables permits control over the range of these variables and immediate response should the level of a critical variable, e.g., reactor temperature or pressure, exceed its safety threshold.

The software packages which have been implemented in support of GC data collection and analysis include programs to achieve input/output, perform peak integration including baseline correction, compute test parameters, list parameters, assemble and store data, generate summary reports, etc. A capability for achieving simultaneous use of two or more GC systems is being developed.

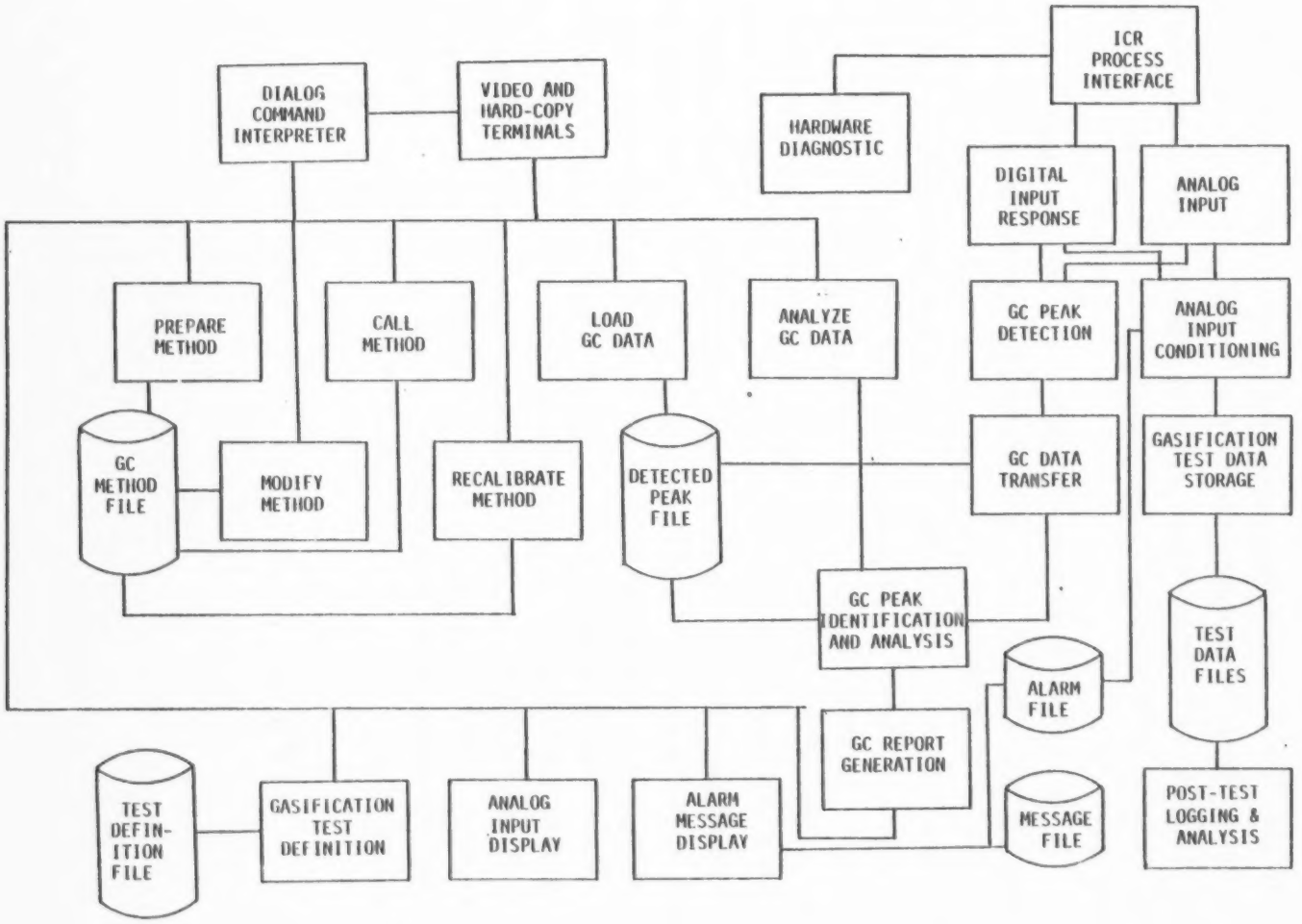

Figure 20. Signal processing software system.

APPENDIX II

POLLUTANT PRODUCTION FACTORS

(g produced/g coal loaded)

TABLE II-1. POLLUTANT PRODUCTION IN COAL GASIFICATION--RUN NO.16: ILLINOIS NO.6 COAL

g produced/g coal loaded

	GAS	CONDENSATE	TAR	TOTAL
H_2S	2.1E-2			2.1E-2
COS	2.2E-4			2.2E-4
CS_2	4.2E-5			4.2E-5
methanethiol	2.2E-5			2.2E-5
ethanethiol				N/A
thiophene	1.0E-3			1.0E-3
methylthiophene	1.8E-4			1.8E-4
ammonia	N/A			N/A
benzene	2.8E-3			2.8E-3
toluene	2.0E-2			2.0E-2
xylenes	4.9E-5			4.9E-5
phenol	1.3E-5	2.2E-4	7.8E-6	2.4E-4
cresols	1.1E-5	3.8E-4	1.9E-5	4.1E-4
xylenols				N/A
chrysene				N/A
perylene				N/A
pyrene	2.5E-7		6.4E-5	6.4E-5
fluorene	1.8E-8		2.7E-6	2.7E-6
anthracene	1.4E-6		3.9E-4	3.9E-4
naphthalene	7.0E-5		6.1E-4	6.8E-4
biphenyl	1.0E-6			1.0E-6
indene	2.3E-4			2.3E-4
benzofuran	3.3E-4			3.3E-4
dibenzofuran			3.2E-7	3.2E-7
aniline				N/A

TABLE II-2. POLLUTANT PRODUCTION IN COAL GASIFICATION--RUN NO.21
ILLINOIS NO.6 COAL

g produced/g coal loaded

	GAS	CONDENSATE	TAR	TOTAL
H_2S	2.2E-2			2.2E-2
COS	1.2E-4			1.2E-4
CS_2	3.0E-5			3.0E-5
methanethiol	5.0E-5			5.0E-5
ethanethiol				N/A
thiophene	3.6E-4			3.6E-4
methylthiophene	6.0E-4			6.0E-4
ammonia	7.8E-4	8.7E-3		9.5E-3
benzene				N/A
toluene				N/A
xylenes	2.6E-4			2.6E-4
phenol	8.3E-5	1.0E-4	9.4E-5	2.8E-4
cresols	2.0E-4	2.4E-4	3.6E-4	8.0E-4
xylenols	2.0E-4	1.5E-4	8.7E-5	4.4E-4
chrysene			2.6E-4	2.6E-4
perylene				N/A
pyrene			2.9E-4	2.9E-4
fluorene			2.6E-4	2.6E-4
anthracene	4.8E-6			4.8E-6
naphthalene	5.0E-4		1.9E-3	2.4E-3
biphenyl	5.6E-6			5.6E-6
indene	5.6E-6			5.6E-6
benzofuran	6.3E-5			6.3E-5
dibenzofuran	3.0E-5		2.4E-4	2.7E-4
aniline			8.7E-6	8.7E-6

TABLE II-3. POLLUTANT PRODUCTION IN COAL GASIFICATION--RUN NO.23
ILLINOIS NO.6 COAL

g produced/g coal loaded

	GAS	CONDENSATE	TAR	TOTAL
H_2S	5.9E-2			5.9E-2
COS	3.4E-4			3.4E-4
CS_2	1.5E-4			1.5E-4
methanethiol	3.1E-5			3.1E-5
ethanethiol	1.3E-6*			1.3E-6
thiophene	2.3E-3			2.3E-3
methylthiophene	6.6E-4			6.6E-4
ammonia				N/A
benzene	8.7E-3			8.7E-3
toluene	3.1E-3			3.1E-3
xylenes	3.8E-4			3.8E-3
phenol	1.3E-4	1.9E-4	1.5E-4	4.7E-4
cresols	3.1E-4	2.4E-4	4.5E-4	1.0E-3
xylenols		9.3E-5	3.5E-4	4.4E-4
chrysene			2.8E-4	2.8E-4
perylene			1.2E-4	1.2E-4
pyrene			3.5E-4	3.5E-4
fluorene			1.5E-5	1.5E-5
anthracene	4.1E-6		2.4E-4	2.4E-4
naphthalene	2.0E-3		8.5E-4	2.9E-3
biphenyl	9.3E-6			9.3E-6
indene	2.2E-4			2.2E-4
benzofuran	1.9E-4			1.9E-4
dibenzofuran	4.1E-5		1.7E-4	2.1E-4
aniline			6.1E-6	

*Includes dimethyl sulfide.

TABLE II-4. POLLUTANT PRODUCTION IN COAL GASIFICATION--RUN NO.41
WESTERN KENTUCKY NO.9

g produced/g coal loaded

	GAS	CONDENSATE	TAR	TOTAL
H_2S	2.7E-2			2.7E-2
COS	5.7E-4			5.7E-4
CS_2	7.5E-7			7.5E-7
methanethiol	3.8E-5			3.8E-5
ethanethiol	1.1E-4*			1.1E-4
thiophene	2.7E-4			2.7E-4
methylthiophene	3.3E-4			3.3E-4
ammonia				N/A
benzene	1.3E-2			1.3E-2
toluene	1.7E-3			1.7E-3
xylenes	2.8E-4			2.8E-4
phenol	3.6E-4	4.2E-4	3.6E-5	8.2E-4
cresols	2.4E-4	3.8E-4	2.6E-4	8.8E-4
xylenols		5.3E-5	1.4E-4	1.9E-4
chrysene				N/A
perylene				N/A
pyrene			7.2E-4	7.2E-4
fluorene			2.3E-4	2.3E-4
anthracene	6.9E-6		6.8E-4	6.8E-4
naphthalene	2.1E-3		2.6E-4	2.7E-3
biphenyl	5.7E-6			5.7E-6
indene	5.0E-4			5.0E-4
benzofuran	1.2E-4			1.2E-4
dibenzofuran	3.5E-6		2.4E-4	2.4E-4
aniline			6.3E-7	6.3E-7

*Includes dimethyl sulfide.

TABLE II-5. POLLUTANT PRODUCTION IN COAL GASIFICATION--RUN NO.25
MONTANA ROSEBUD COAL

g produced/g coal loaded

	GAS	CONDENSATE	TAR	TOTAL
H_2S	2.5E-3			2.5E-3
COS	8.0E-5			8.0E-5
CS_2				N/A
methanethiol	2.2E-6			2.2E-6
ethanethiol				N/A
thiophene	2.8E-5			2.8E-5
methylthiophene	5.9E-6			5.9E-6
ammonia	5.9E-4	4.2E-3		4.8E-3
benzene	3.6E-4			3.6E-3
toluene	5.4E-4			5.4E-4
xylenes	4.8E-4			4.8E-4
phenol	8.0E-5	2.6E-4	7.6E-5	4.2E-4
cresols	2.8E-5	1.1E-4	1.4E-4	2.8E-4
xylenols	5.6E-5	9.6E-6	4.1E-5	1.1E-4
chrysene			1.3E-4	1.3E-4
perylene			4.8E-4	4.8E-4
pyrene			1.8E-4	1.8E-4
fluorene			1.3E-4	1.3E-4
anthracene	1.6E-6		1.1E-4	1.1E-4
naphthalene	1.0E-4		2.1E-4	3.1E-4
biphenyl	1.6E-6			1.6E-6
indene	8.3E-5			8.3E-5
benzofuran	2.6E-5			2.6E-5
dibenzofuran	2.3E-6		9.6E-5	9.8E-5
aniline			6.8E-7	6.8E-7

TABLE II-6. POLLUTANT PRODUCTION IN COAL GASIFICATION--RUN NO.33
WYOMING SUBBITUMINOUS COAL

g produced/g coal loaded

	GAS	CONDENSATE	TAR	TOTAL
H_2S	1.9E-3			1.9E-3
COS	1.1E-4			1.1E-4
CS_2				N/A
methanethiol	1.4E-5			1.4E-5
ethanethiol				N/A
thiophene	9.1E-6			9.1E-6
methylthiophene	1.0E-4			1.0E-4
ammonia				N/A
benzene	4.6E-3			4.6E-3
toluene	1.8E-3			1.8E-3
xylenes	4.6E-4			4.6E-4
phenol	1.2E-3	1.3E-4	1.6E-4	1.5E-3
cresols	3.3E-4	1.4E-4	3.5E-5	5.1E-4
xylenols	1.4E-3	5.1E-5	2.7E-4	1.7E-3
chrysene			2.0E-5	2.0E-5
perylene			1.3E-5	1.3E-5
pyrene			2.6E-5	2.6E-5
fluorene			5.7E-5	5.7E-5
anthracene	2.4E-6		8.3E-5	8.5E-5
naphthalene	2.6E-4		8.9E-5	3.5E-4
biphenyl	6.3E-6			6.3E-6
indene	5.5E-4			5.5E-4
benzofuran				N/A
dibenzofuran	1.8E-5		4.1E-5	5.9E-5
aniline			8.7E-7	8.7E-7

TABLE II-7. POLLUTANT PRODUCTION IN COAL GASIFICATION--RUN NO.35
WYOMING SUBBITUMINOUS COAL

g produced/g coal loaded

	GAS	CONDENSATE	TAR	TOTAL
H_2S	3.8E-3			3.8E-3
COS	2.0E-4			2.0E-4
CS_2				N/A
methanethiol	2.5E-5			2.3E-5
ethanethiol				N/A
thiophene	3.0E-5			3.0E-5
methylthiophene	3.0E-5			3.0E-5
ammonia				N/A
benzene	3.8E-3			3.8E-3
toluene	2.2E-3			2.2E-3
xylenes	8.0E-4			8.0E-4
phenol	6.0E-4	6.8E-4	3.2E-4	1.6E-3
cresols	2.8E-4	4.1E-4	7.8E-4	1.5E-3
xylenols	7.1E-4	8.5E-5	4.9E-4	1.3E-3
chrysene			2.0E-5	2.0E-5
perylene			6.9E-6	6.9E-6
pyrene			3.5E-5	3.5E-5
fluorene			4.9E-5	4.9E-5
anthracene	1.2E-6		7.6E-5	7.7E-5
naphthalene	8.5E-5		4.7E-5	1.3E-4
biphenyl	3.0E-6			3.0E-6
indene	1.4E-4			1.4E-4
benzofuran	1.0E-4			1.0E-4
dibenzofuran	7.3E-6		4.1E-5	4.8E-5
aniline			1.4E-6	1.4E-6

TABLE II-8. POLLUTANT PRODUCTION IN COAL GASIFICATION--RUN NO.36
NORTH DAKOTA ZAP LIGNITE

g produced/g coal loaded

	GAS	CONDENSATE	TAR	TOTAL
H_2S	2.3E-3			2.8E-3
COS	1.7E-4			1.7E-4
CS_2				N/A
methanethiol	7.9E-5			7.9E-5
ethanethiol	2.2E-5*			2.2E-5
thiophene	5.1E-4			5.1E-4
methylthiophene	1.3E-5			1.3E-5
ammonia				N/A
benzene	5.1E-3			5.4E-3
toluene	1.4E-3			1.4E-3
xylenes	3.9E-4			3.9E-4
phenol	1.6E-4	4.7E-4	4.7E-5	6.8E-4
cresols	1.4E-4	2.5E-4	9.1E-5	4.8E-4
xylenols	4.9E-4	6.2E-5	7.1E-6	5.6E-4
chrysene			2.2E-5	2.2E-5
perylene			6.9E-6	6.9E-6
pyrene			4.0E-5	4.0E-5
fluorene			4.0E-5	4.0E-5
anthracene	9.3E-7		1.0E-4	1.0E-4
naphthalene	2.3E-4		1.8E-5	2.5E-4
biphenyl	3.2E-6			3.2E-6
indene	7.9E-5			7.9E-5
benzofuran	1.4E-5			1.4E-5
dibenzofuran			3.1E-5	3.1E-5
aniline				N/A

*Includes dimethyl sulfide.

TABLE II-9: POLLUTANT PRODUCTION IN COAL GASIFICATION--RUN NO.43
NORTH DAKOTA ZAP LIGNITE

g produced/g coal loaded

	GAS	CONDENSATE	TAR	TOTAL
H_2S	1.4E-3			1.4E-3
COS	2.7E-4			2.7E-4
CS_2	6.7E-6			6.7E-6
methanethiol	1.1E-5			1.1E-5
ethanethiol	1.3E-5*			1.3E-5
thiophene	8.9E-6			8.9E-6
methylthiophene	3.5E-5			3.5E-5
ammonia				N/A
benzene	1.6E-3			1.6E-3
toluene	9.1E-4			9.1E-4
xylenes	2.9E-4			2.9E-4
phenol	1.9E-5	1.2E-3	3.7E-5	1.3E-3
cresols	1.1E-4	6.9E-4	1.2E-4	9.2E-4
xylenols	8.1E-7	1.4E-4	8.7E-4	1.0E-3
chrysene			4.2E-5	4.2E-5
perylene			6.3E-7	6.3E-7
pyrene			9.5E-6	9.5E-6
fluorene			2.9E-5	2.9E-5
anthracene	4.0E-6		4.9E-5	5.3E-5
naphthalene	5.1E-5		2.6E-5	7.7E-5
biphenyl	2.1E-6			2.1E-6
indene	2.2E-4			2.2E-4
benzofuran	6.3E-5			6.3E-5
dibenzofuran	7.7E-7		3.4E-5	3.4E-5
aniline			2.7E-8	2.7E-8